

Supporting information: Phase field crystal modeling of graphene/hexagonal boron nitride interfaces

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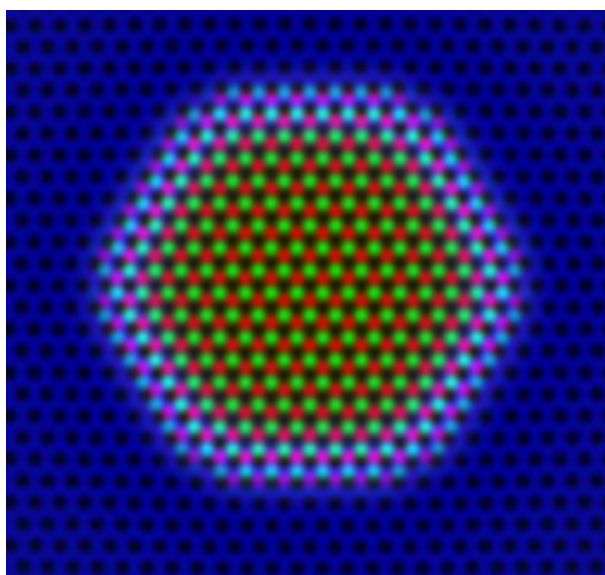
Contents:

1. Hexagonal h-BN crystals with single and multiple layers
2. Multilayered jagged triangular crystals

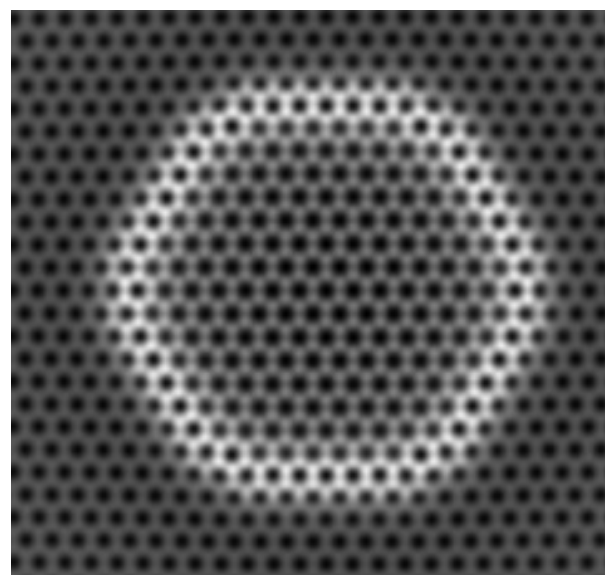
1. Hexagonal h-BN crystals with single and multiple layers

In the following examples, the values for the interfacial couplings, i.e., $\alpha_{C,B}$, $\alpha_{B,C}$, $\alpha_{C,N}$ and $\alpha_{N,C}$ and the third order coupling coefficients, i.e., $\gamma_{C,B}$, $\gamma_{B,C}$, $\gamma_{C,N}$ and $\gamma_{N,C}$ was same. However, the values for the average density of liquid state of h-BN, $\psi_{BN,liquid}$ and the average density of solid state of h-BN, $\psi_{BN,solid}$ were increased in comparison to the average density of liquid state of graphene, $\psi_{C,liquid}$ and the average density of solid state of graphene, $\psi_{C,solid}$. This resulted in the formation of different hexagonal shaped h-BN crystals. This includes crystals having a few atoms to multiple layers on the corners and on the edges.

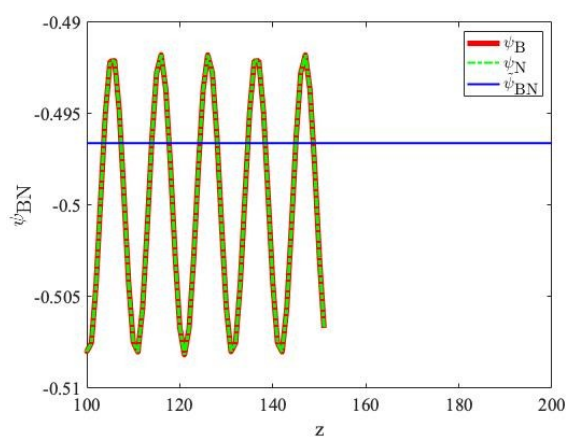
S.1. Example 1



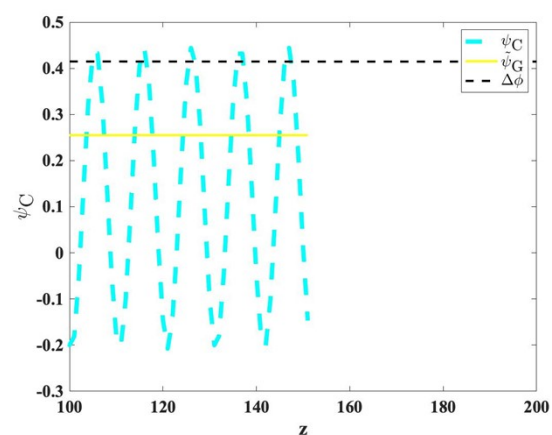
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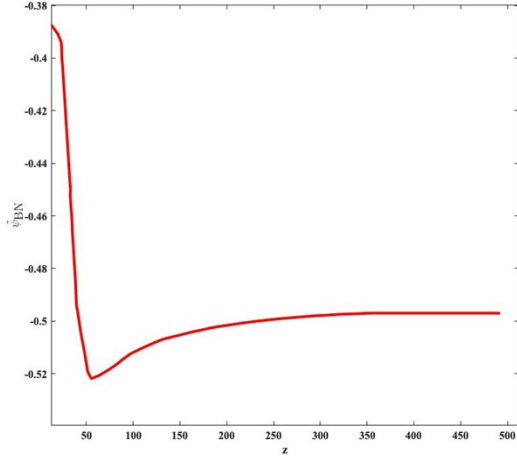
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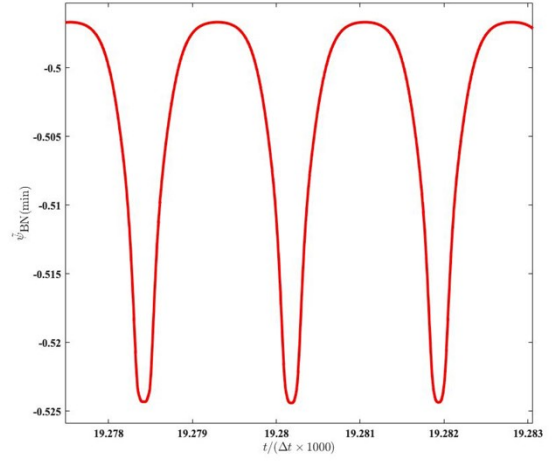
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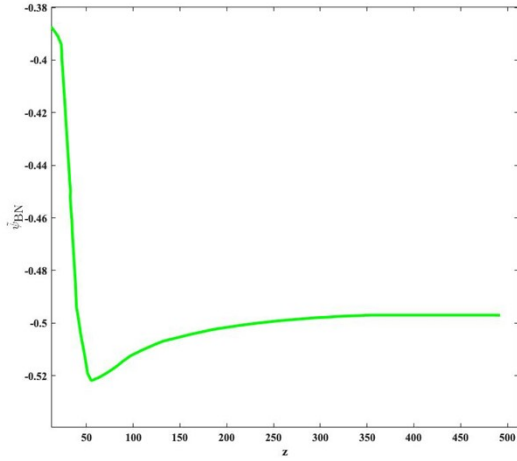
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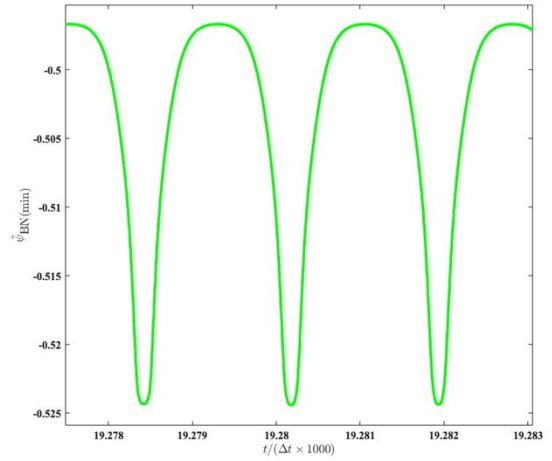
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f.



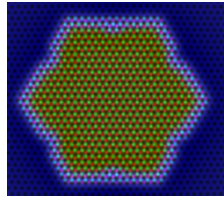
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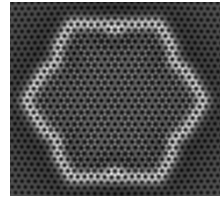
h.

FIG. S.1.(a) h-BN crystal formed at $10000\Delta t$. The carbon, boron and nitrogen atoms are represented by blue, red and green colors, respectively, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, Z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$. Here, τ is the dimensionless time, and t is time step from 9100 to 10000.

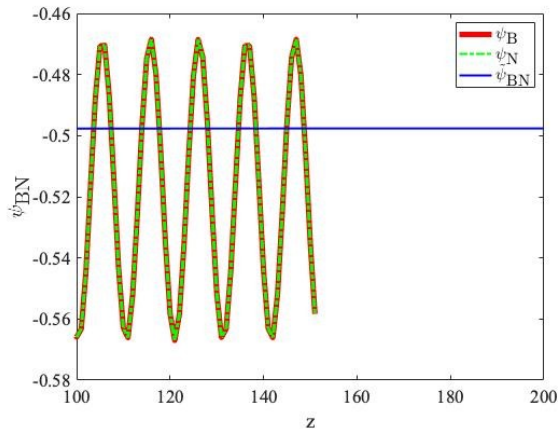
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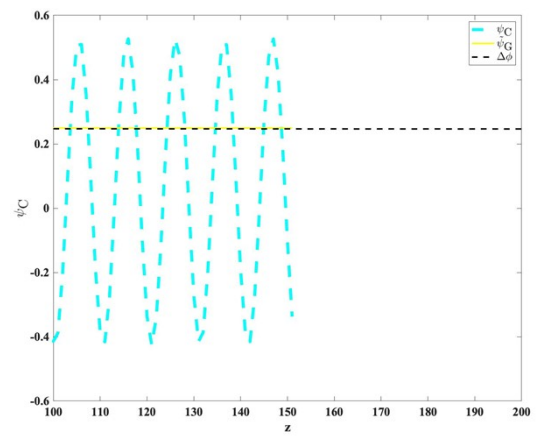
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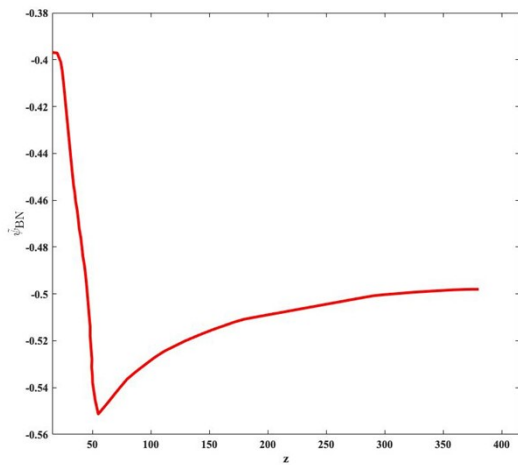
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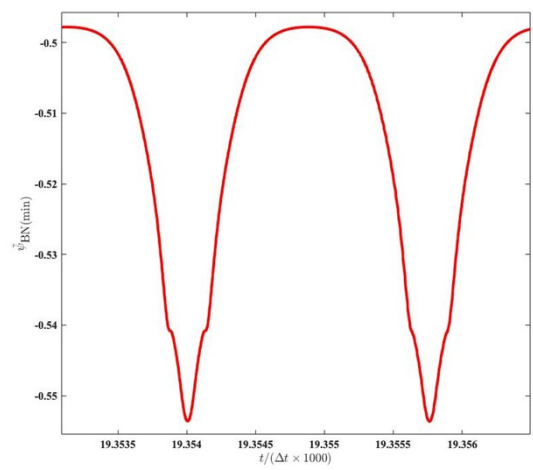
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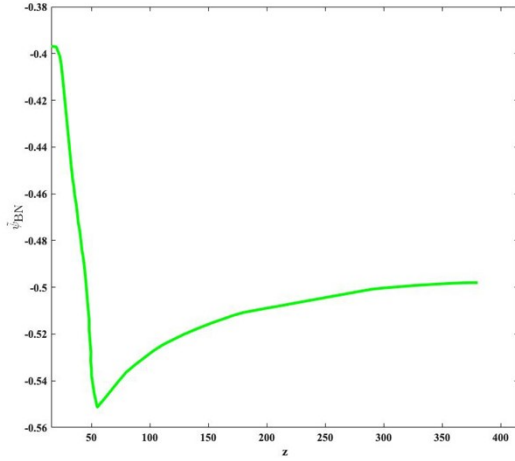
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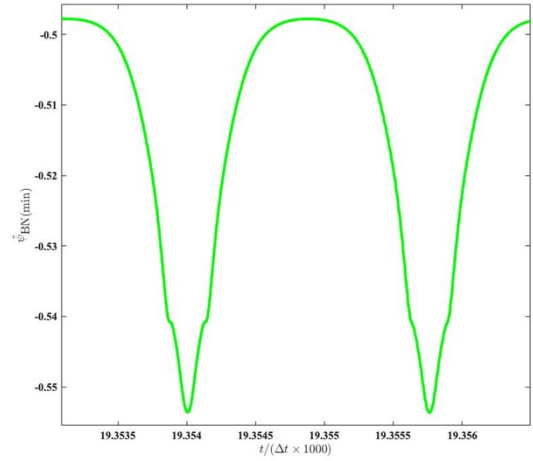
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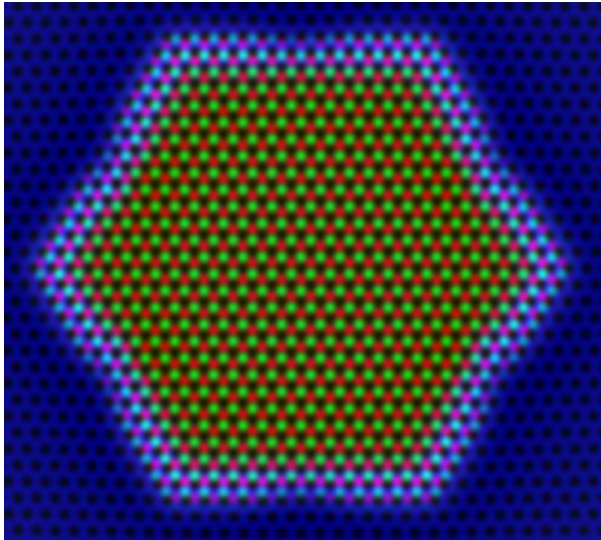
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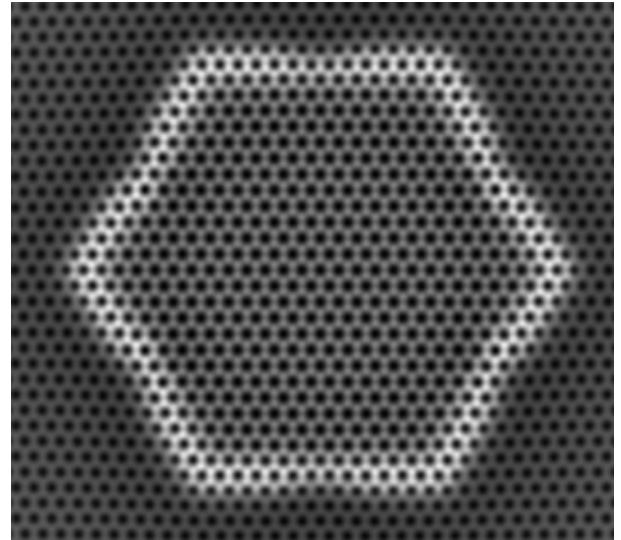
h.

FIG. S.2. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

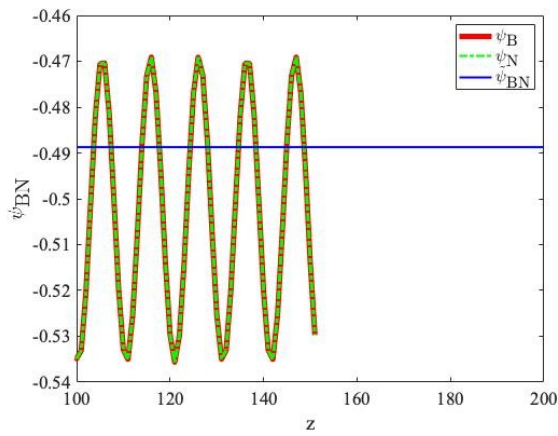
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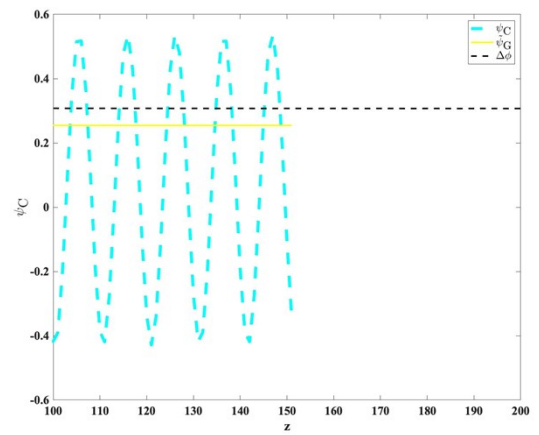
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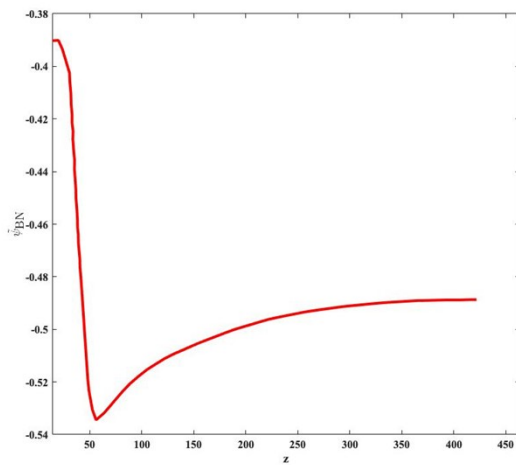
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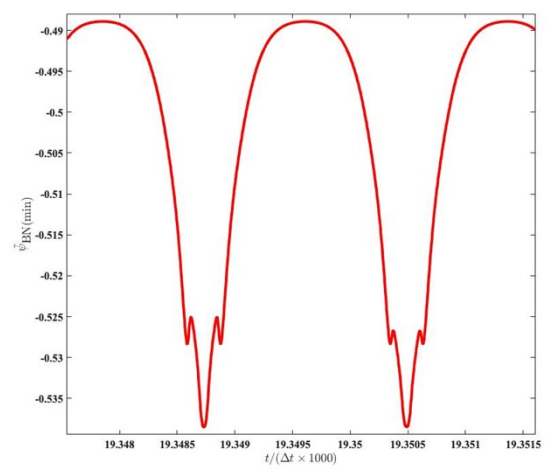
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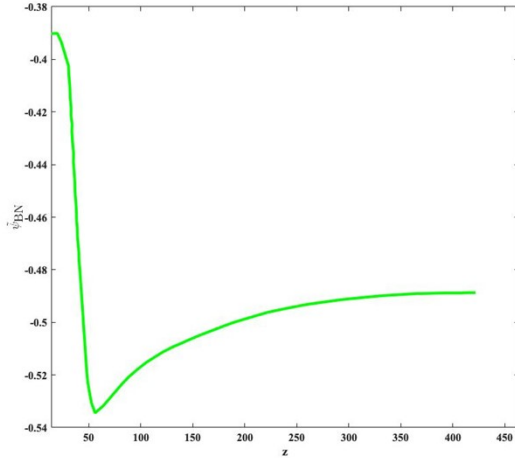
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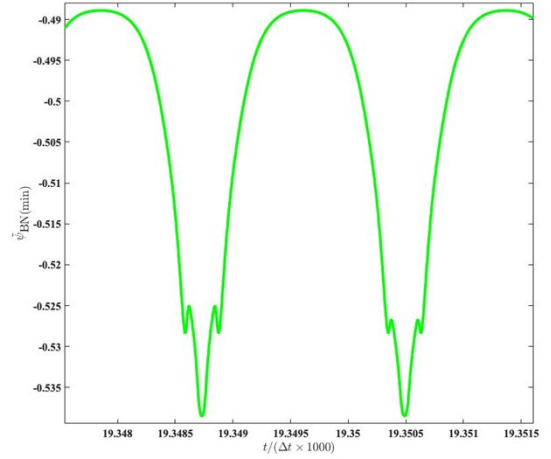
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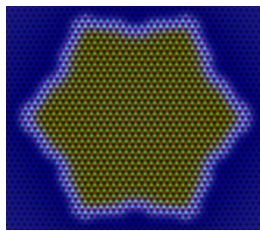
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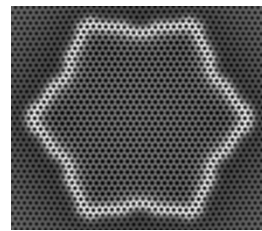
h.

FIG. S.3. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

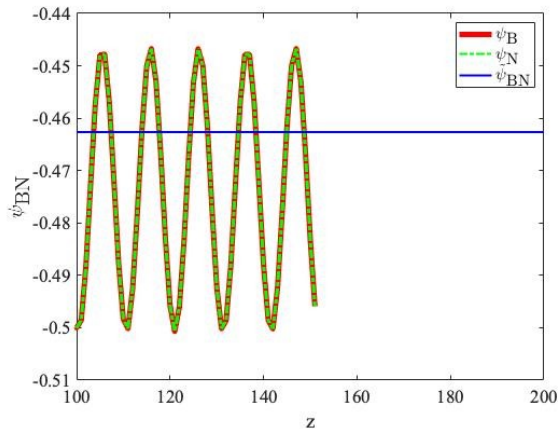
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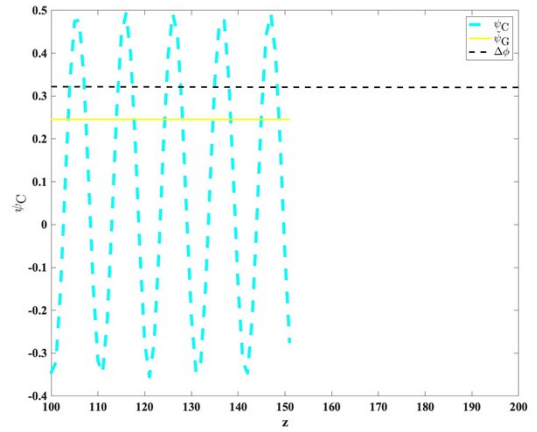
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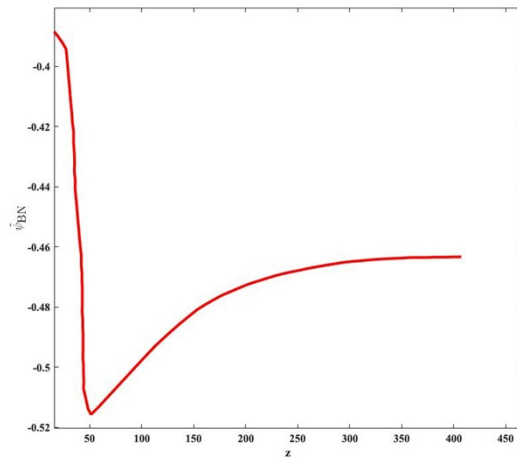
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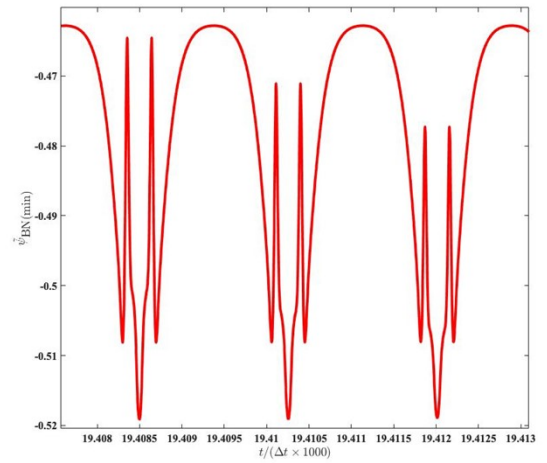
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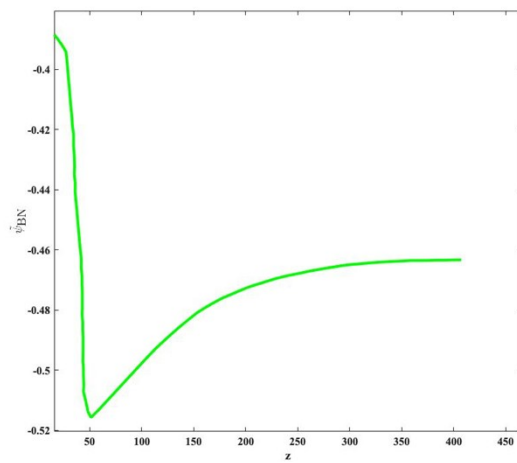
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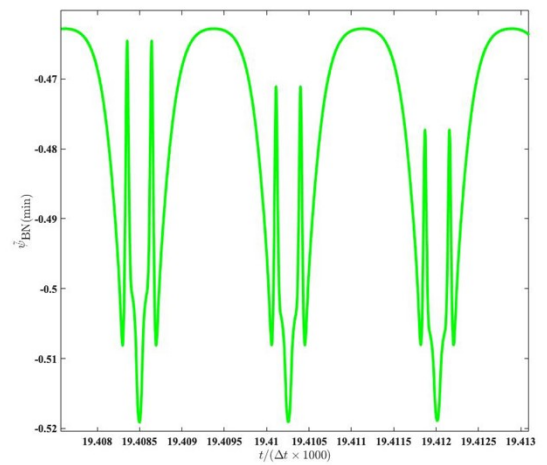
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f.



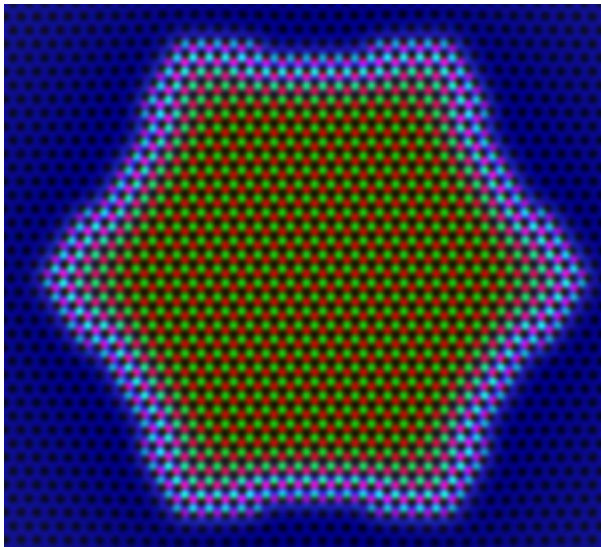
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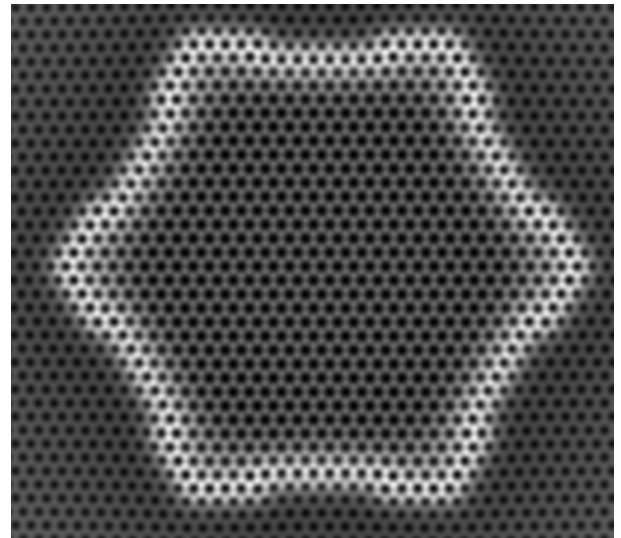
h.

FIG. S.4. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

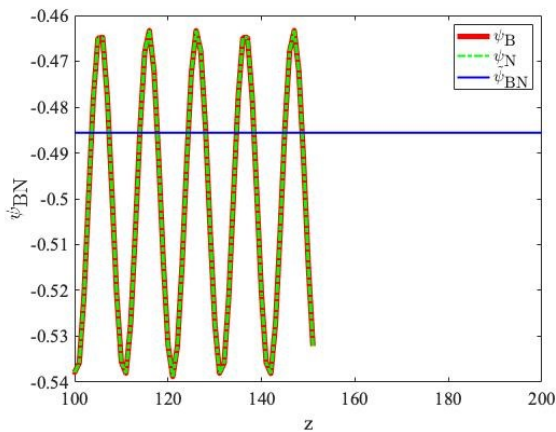
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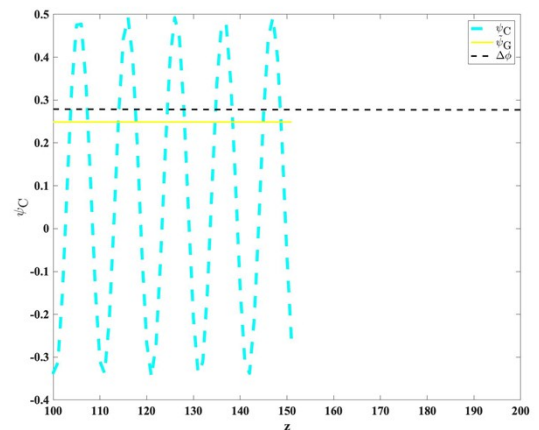
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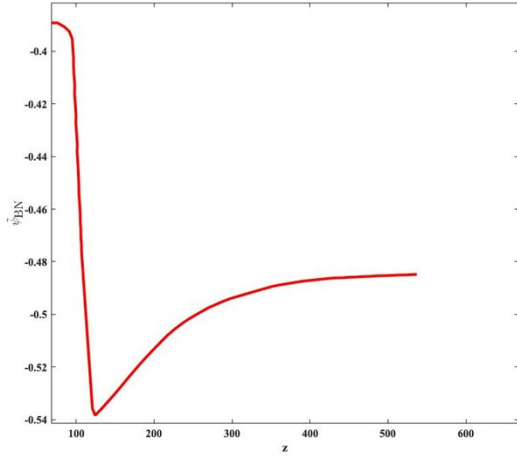
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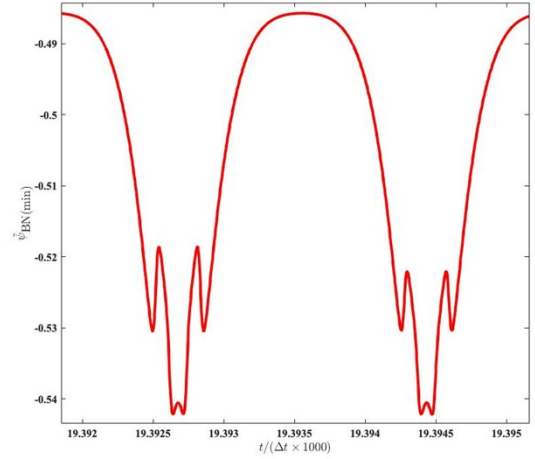
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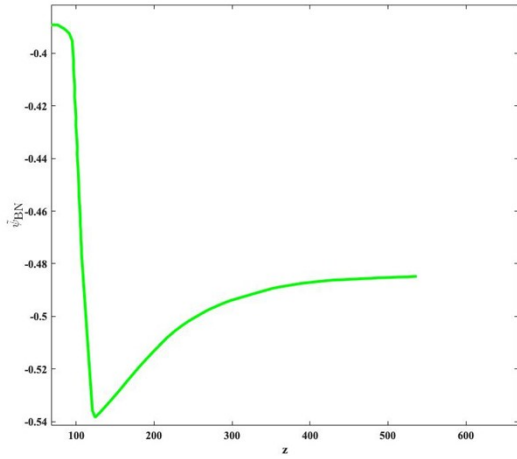
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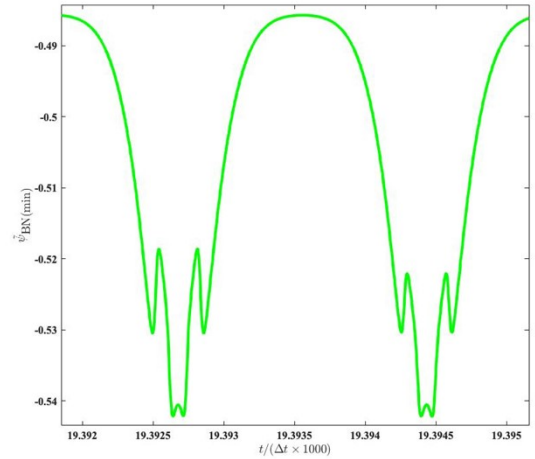
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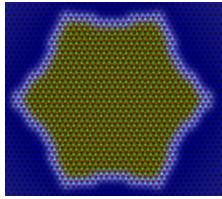
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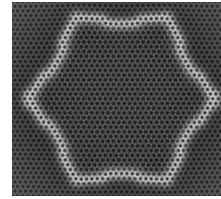
h.

FIG. S.5. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

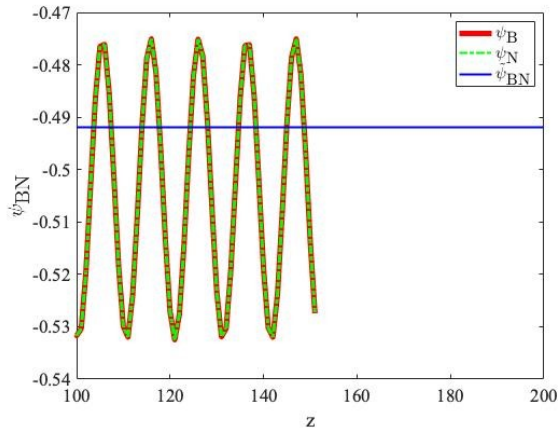
S.6. Example 6



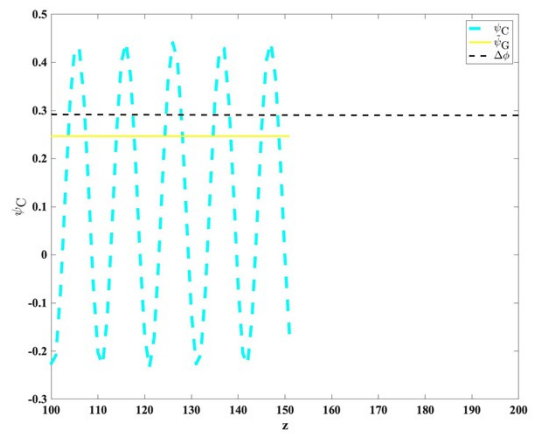
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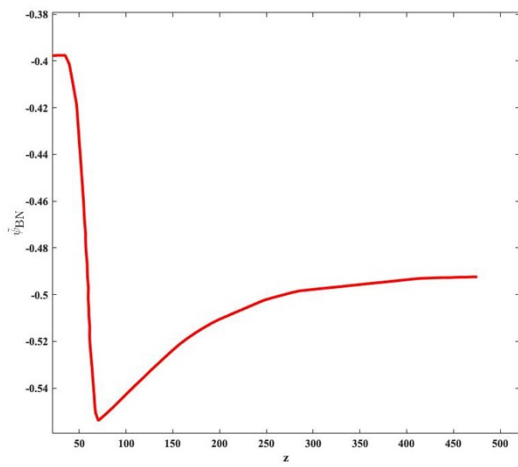
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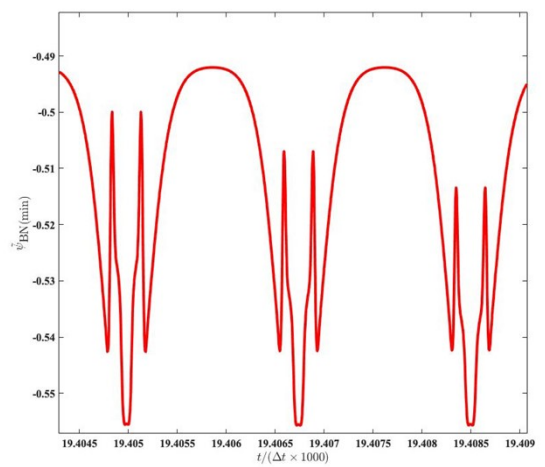
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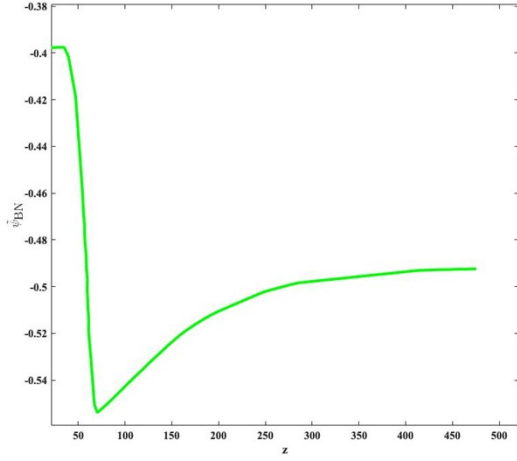
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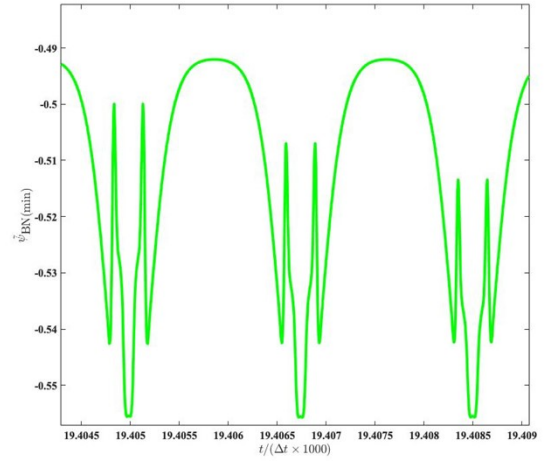
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f.



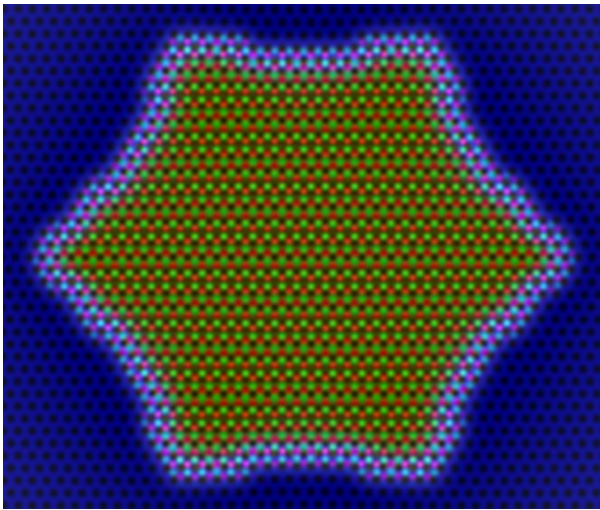
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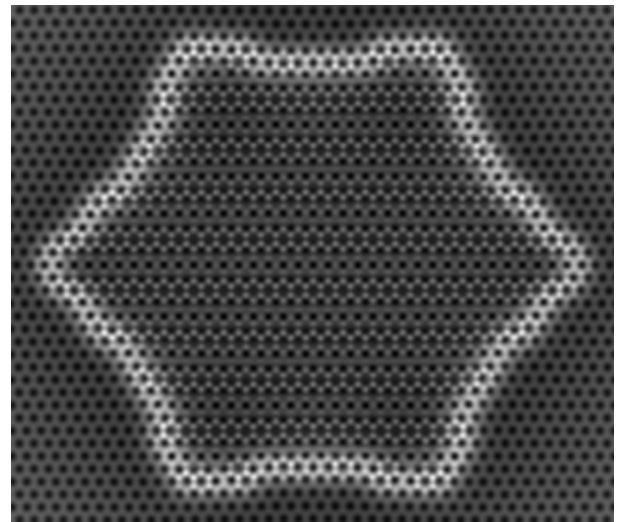
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FIG. S.6. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

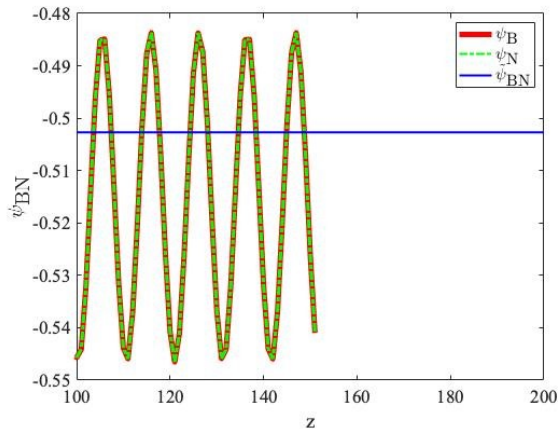
S.7. Example 7



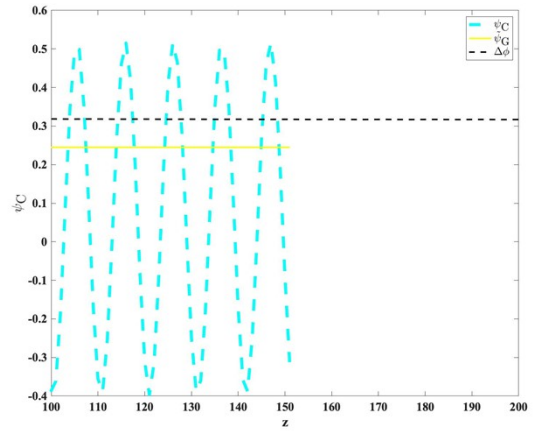
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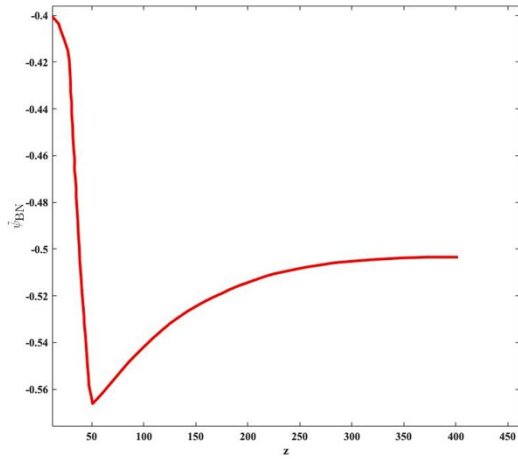
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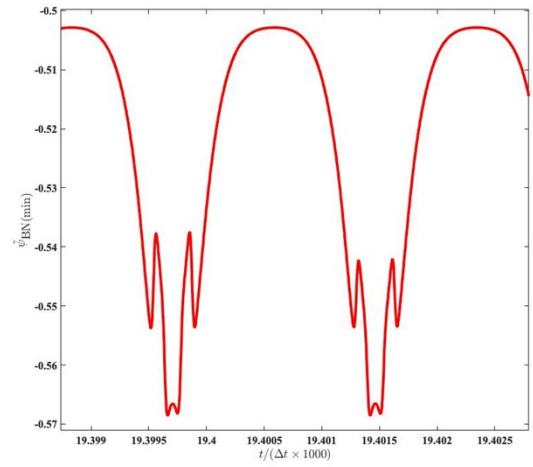
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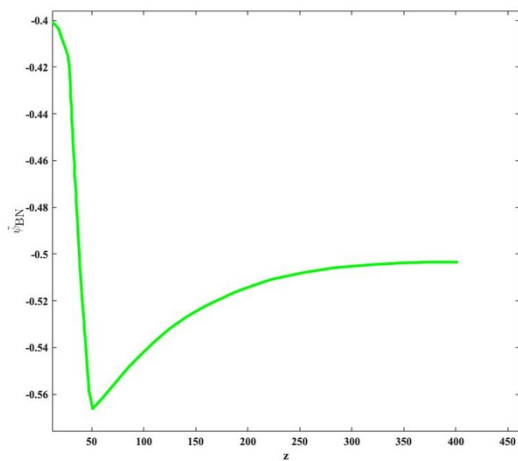
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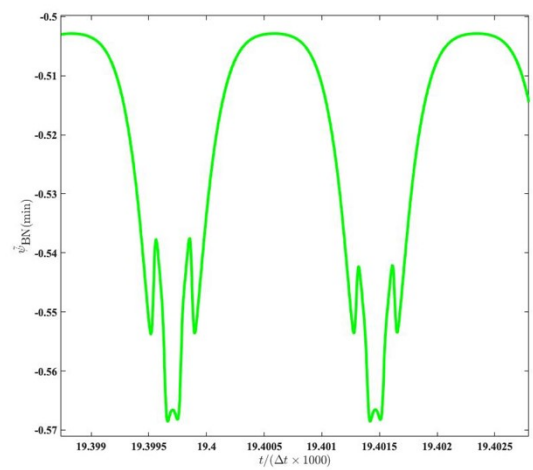
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f.



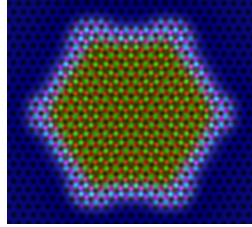
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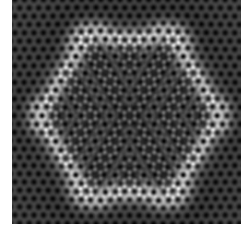
h.

FIG. S.7. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

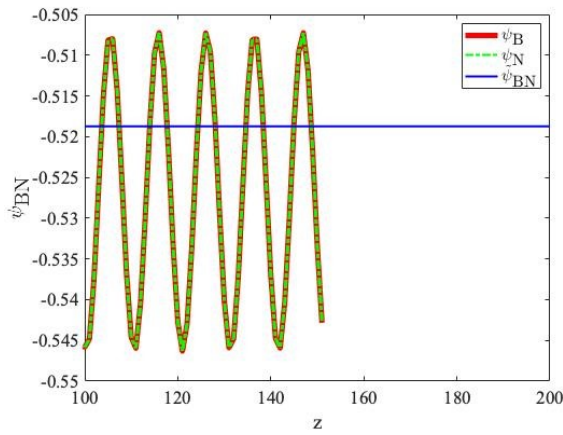
S.8. Example 8



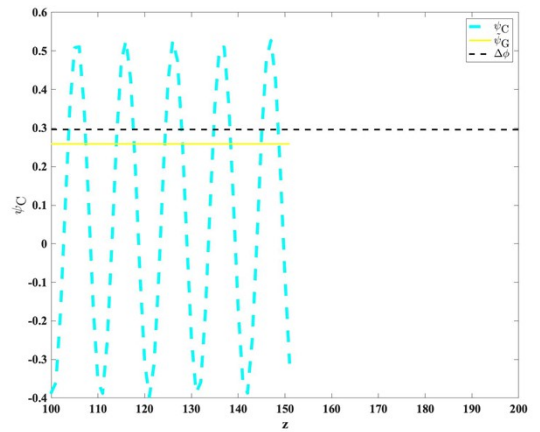
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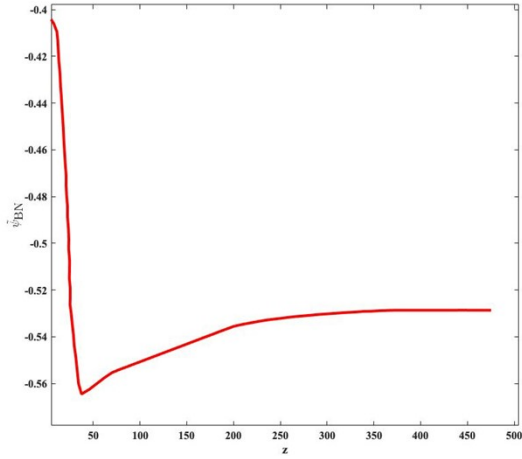
b.



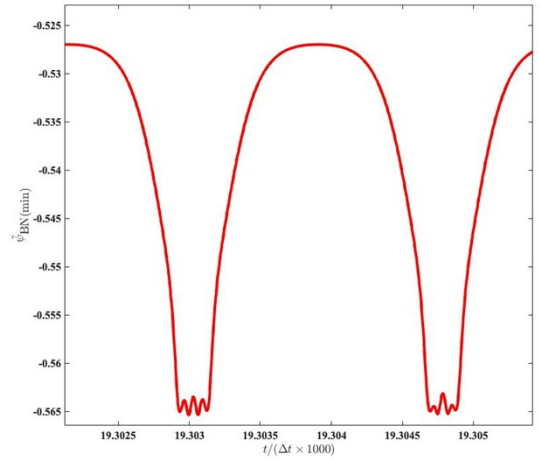
c.



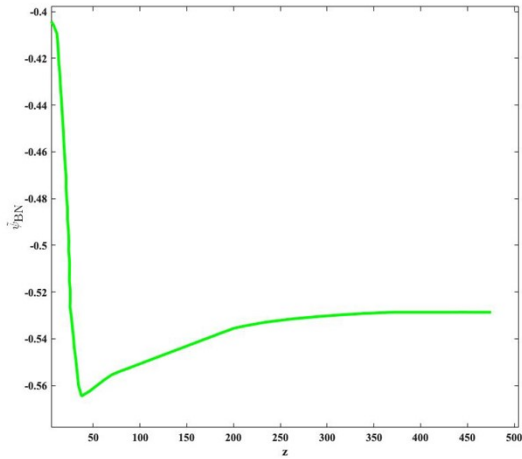
d.



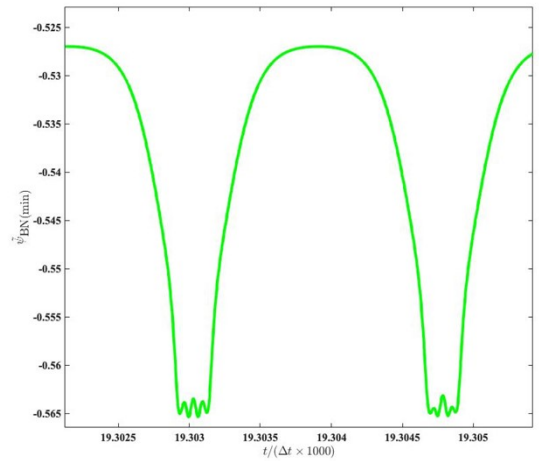
e.



f.



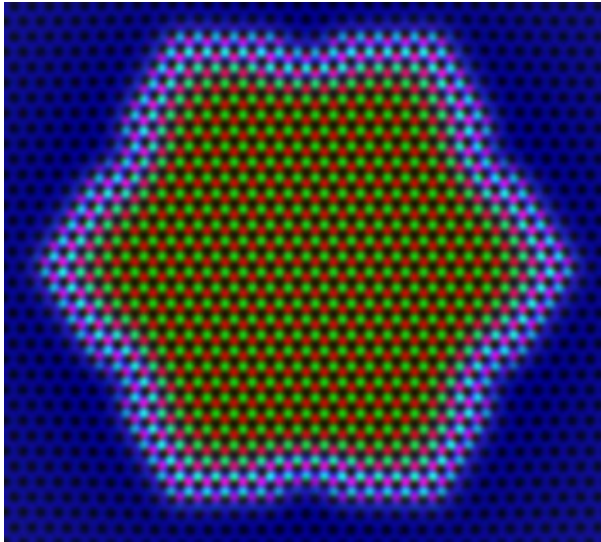
g.



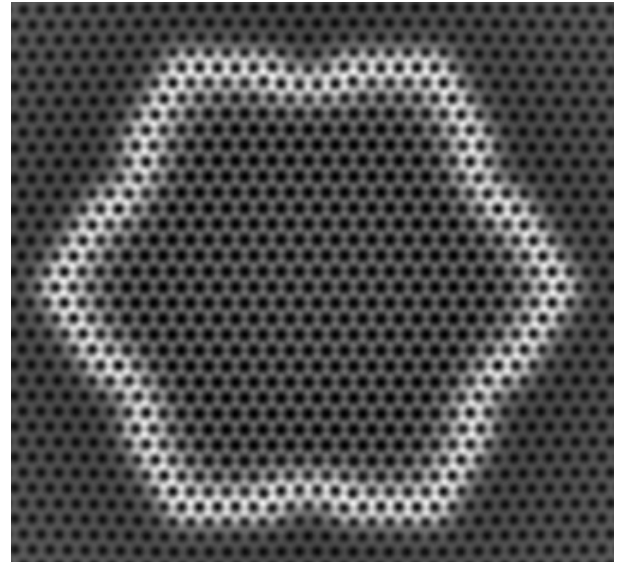
h.

FIG. S.8. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

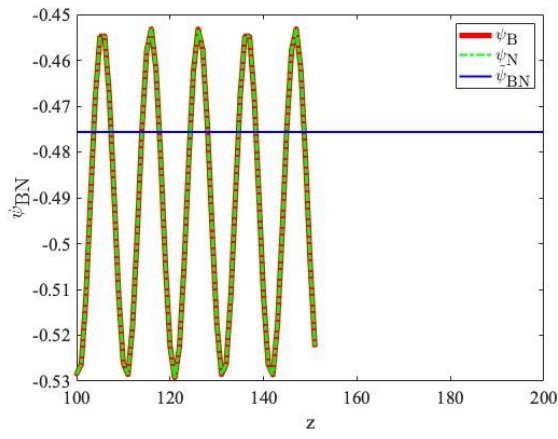
S.9. Example 9



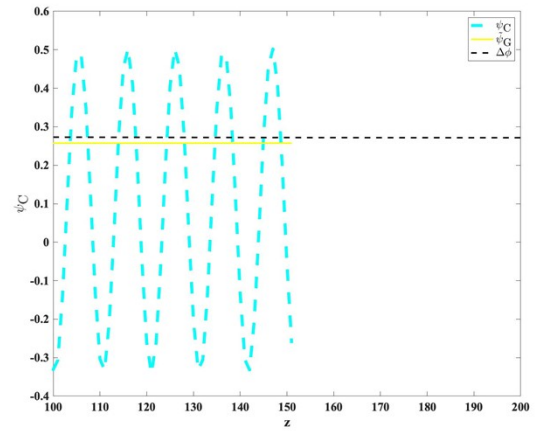
a.



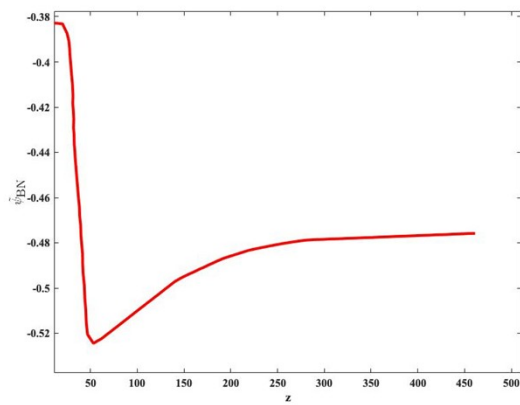
b.



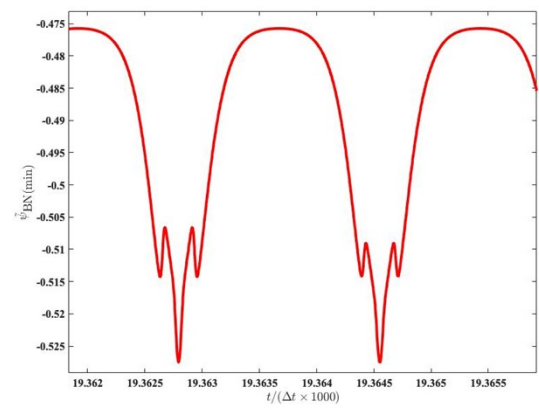
c.



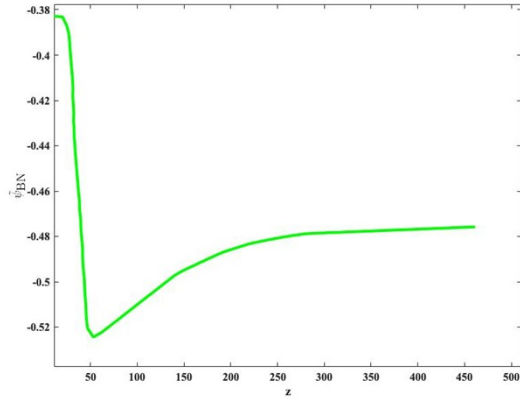
d.



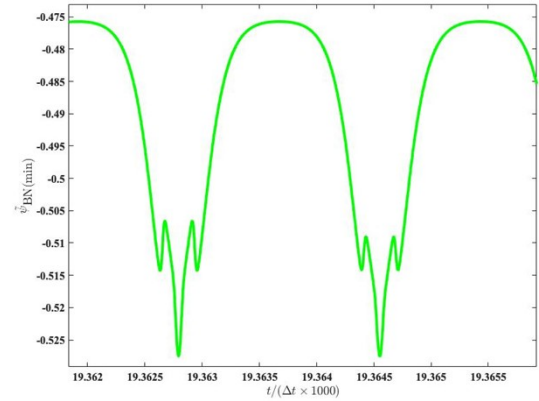
e.



f.



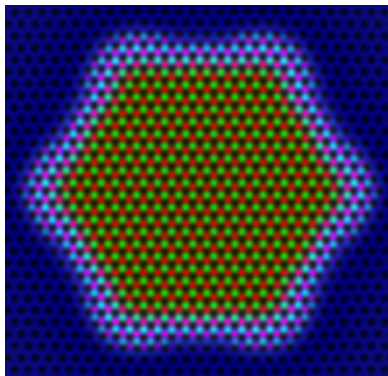
g.



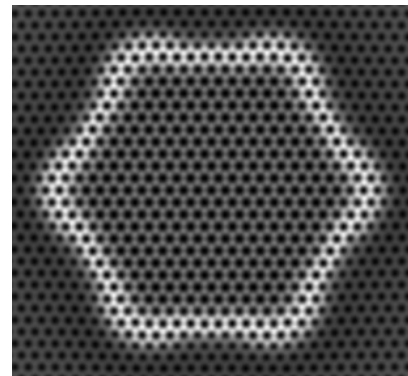
h.

FIG. S. 9. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN}^{(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN}^{(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

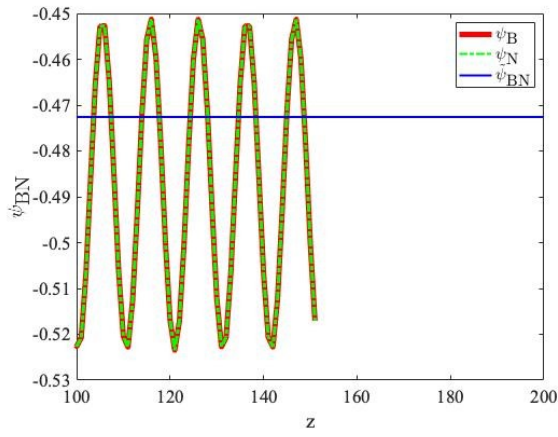
S10. Example 10



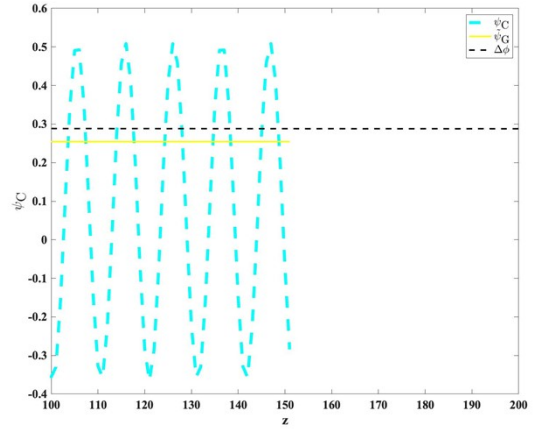
a.



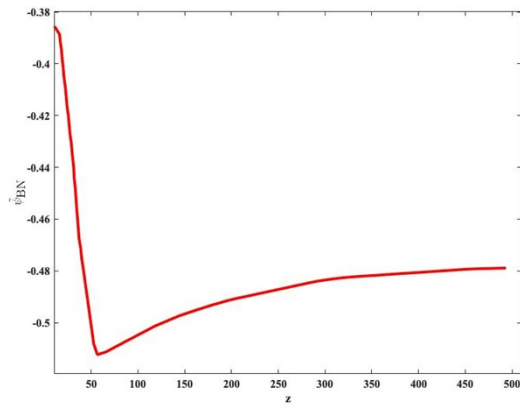
b.



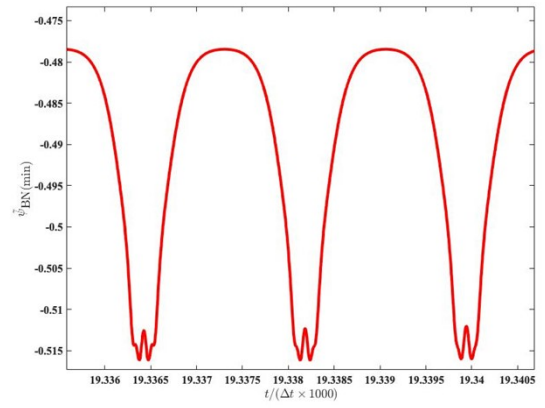
c.



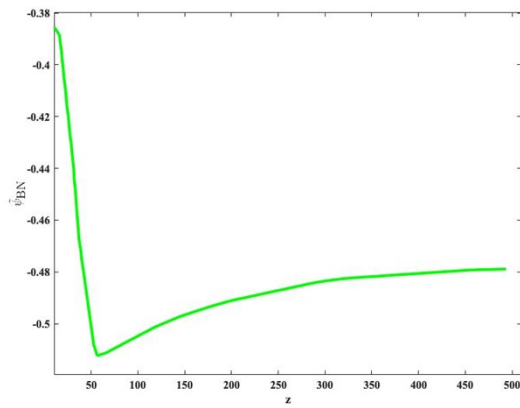
d.



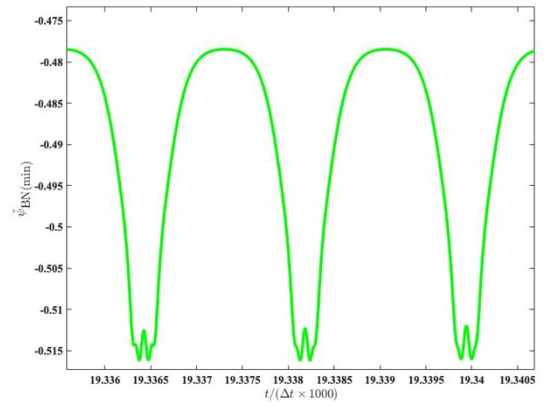
e.



f.



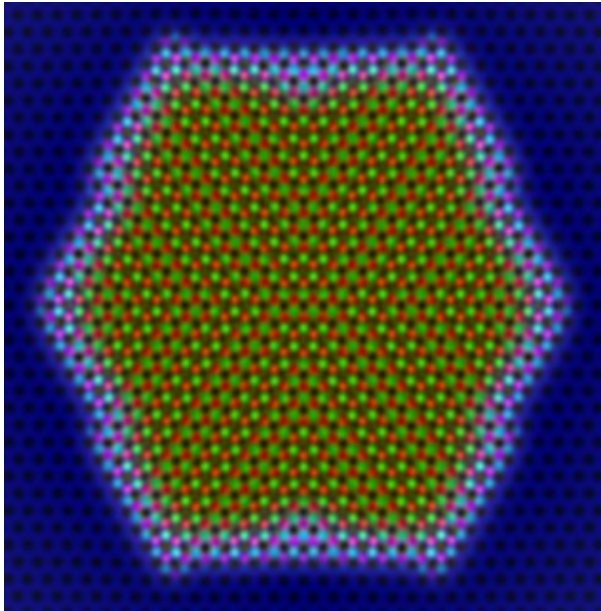
g.



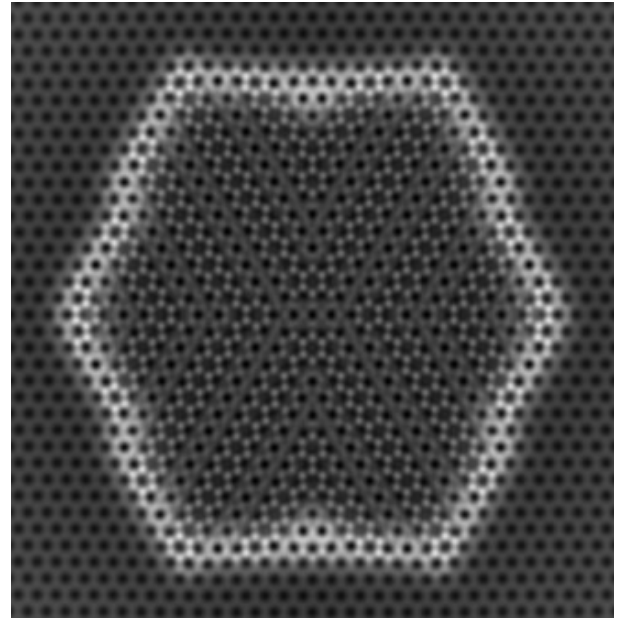
h.

FIG. S. 10. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

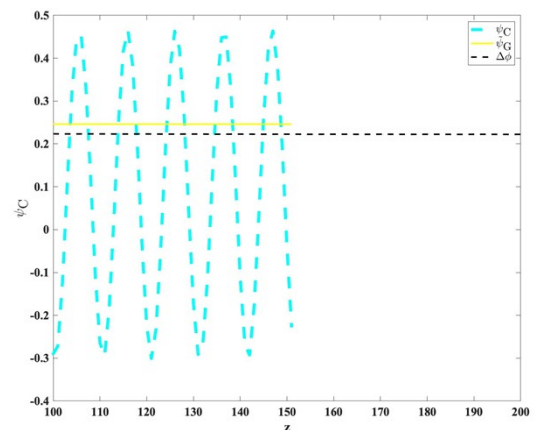
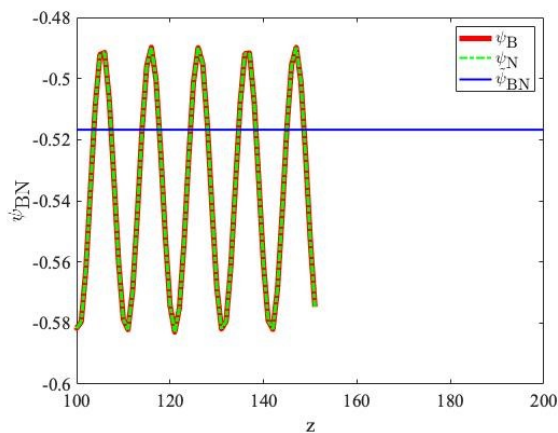
S.11. Example 11



a.



b.



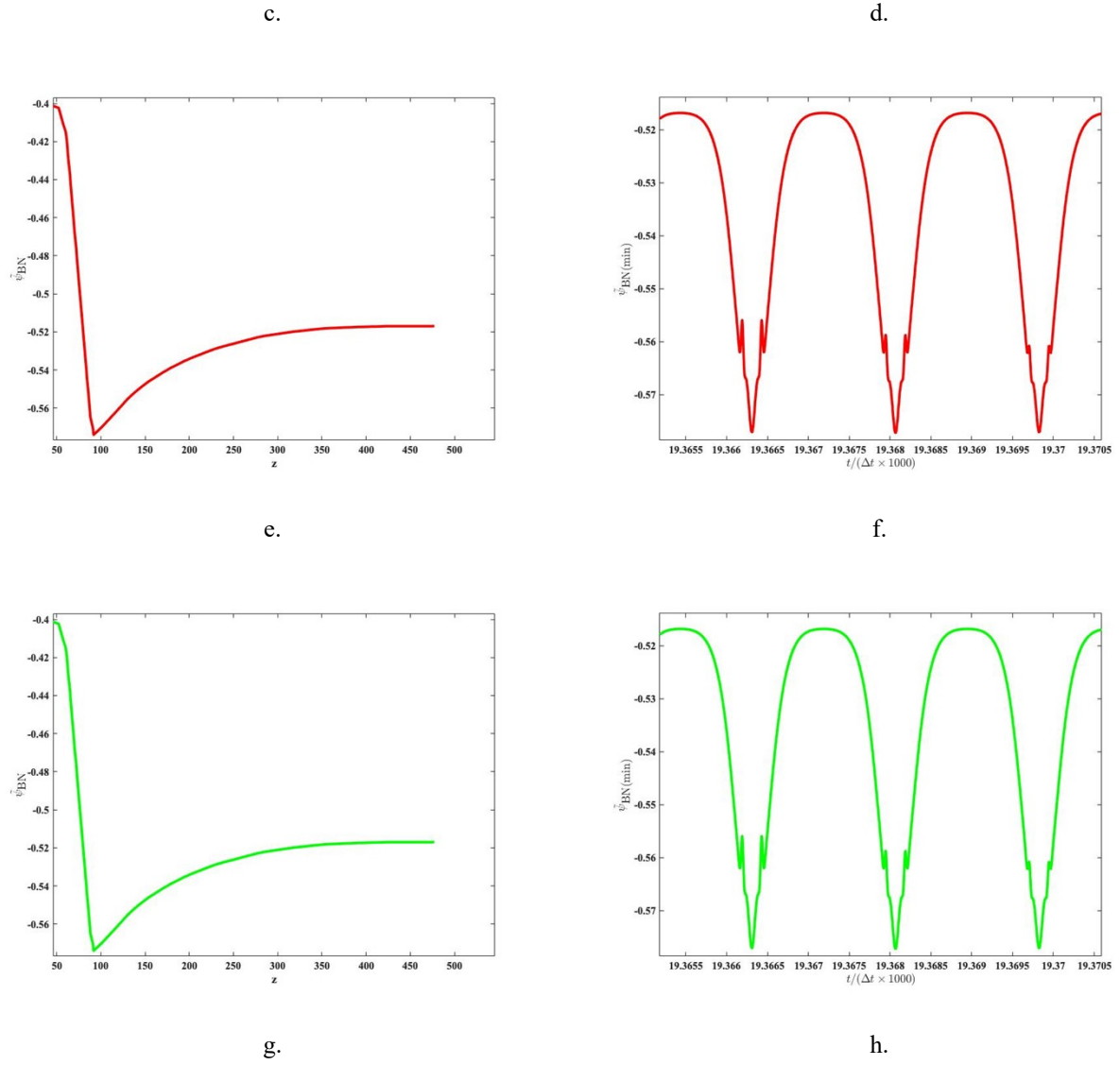
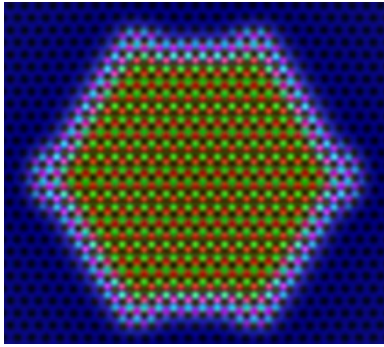
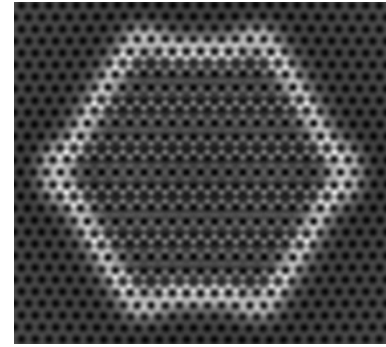


FIG. S.11. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

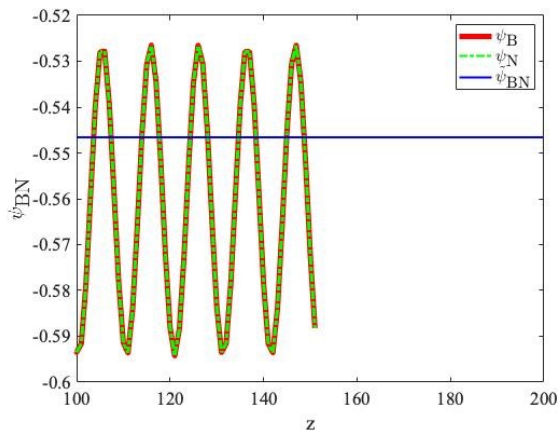
S.12. Example 12



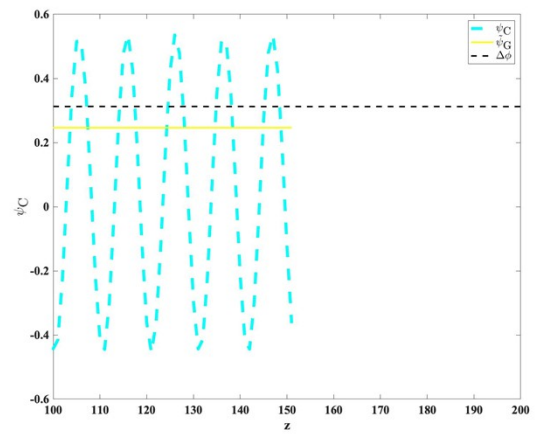
a.



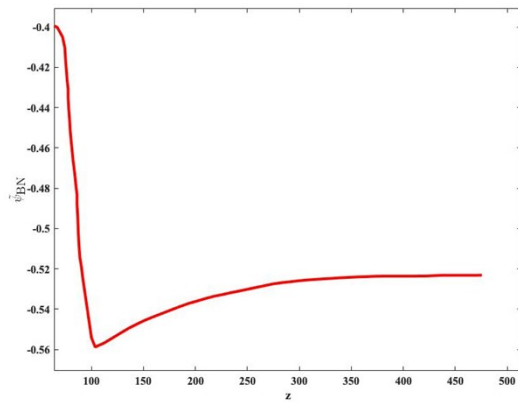
b.



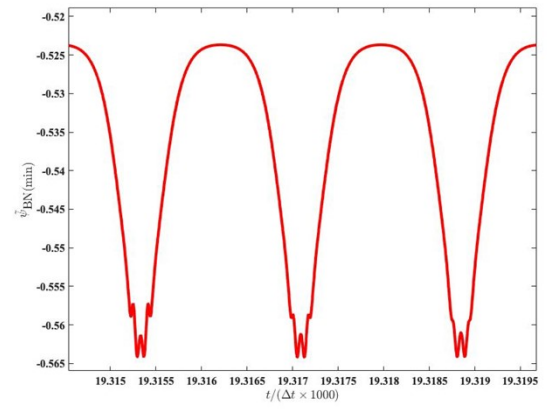
c.



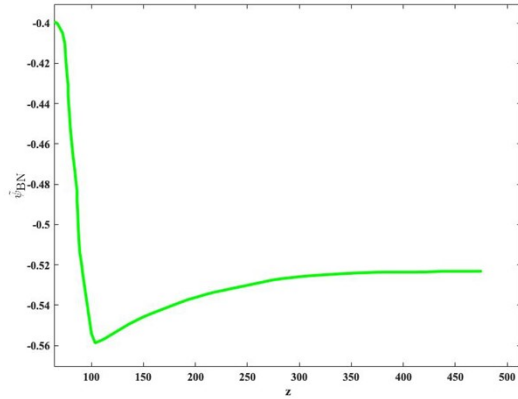
d.



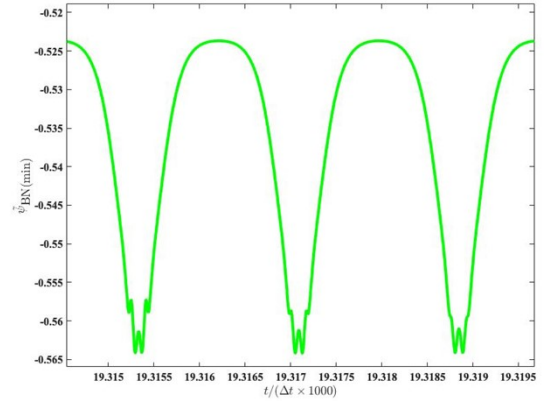
e.



f.



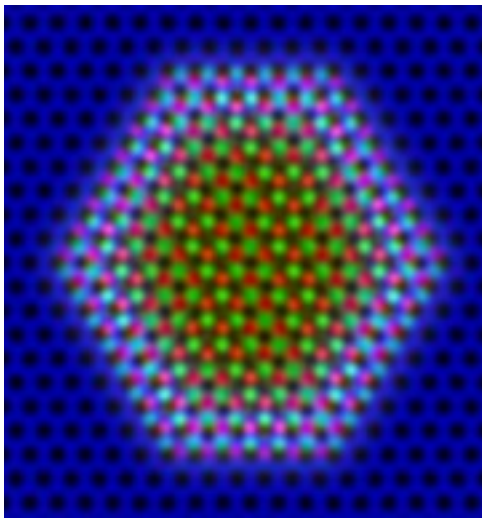
g.



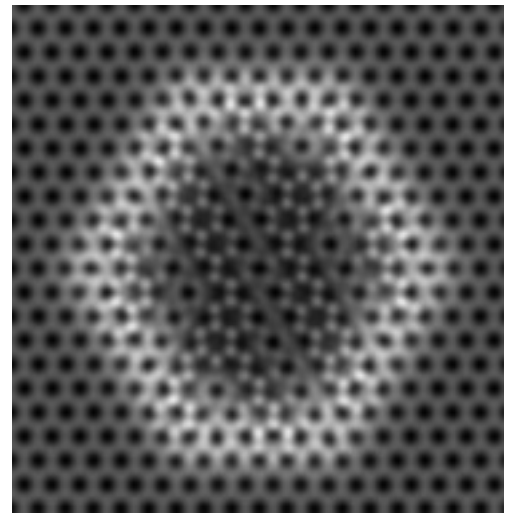
h.

FIG. S. 12. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

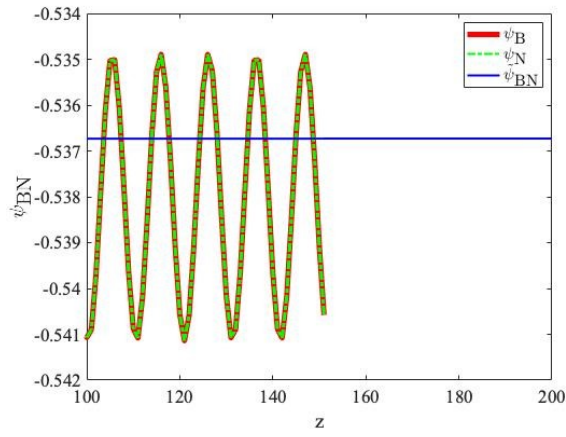
S.13. Example 13



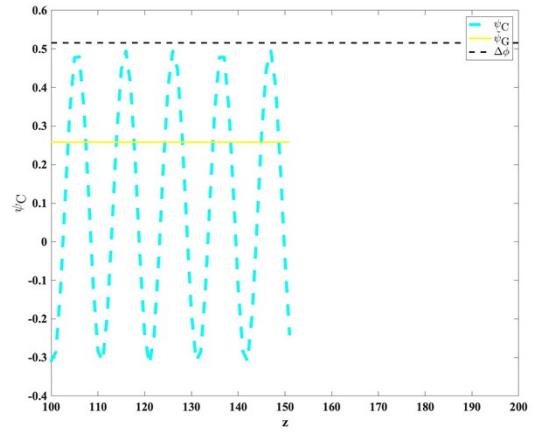
a.



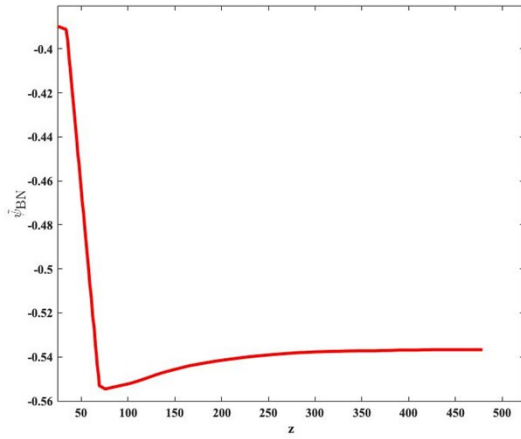
b.



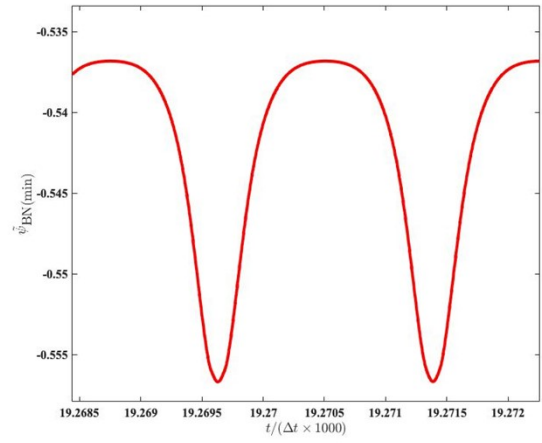
c.



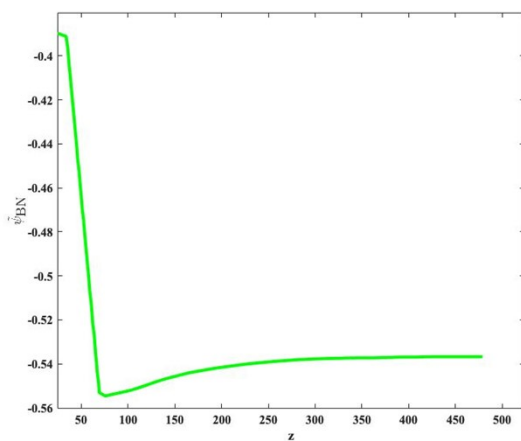
d.



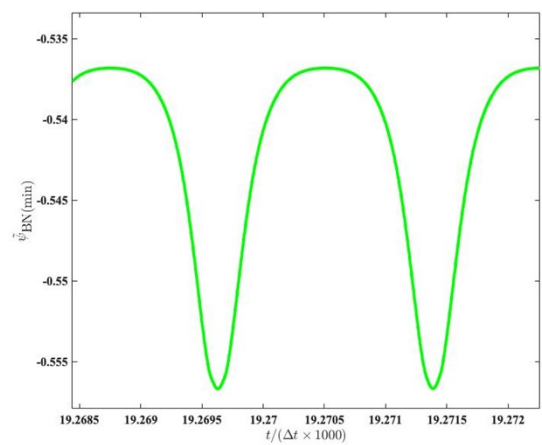
e.



f.



g.



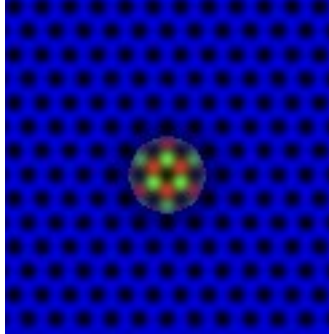
h.

FIG. S. 13. (a) h-BN crystal formed at $10000\Delta t$, (b) the density map of the h-BN crystal at $10000\Delta t$ given in Fig. (a), (c) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front. Here, z is the distance from the center of the particle, along the horizontal center line of the cluster, (d) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (e) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having boron atoms at $10000\Delta t$, (f) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the boron atoms at $10000\Delta t$, (g) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface for different values of the hexagonal shape of h-BN having nitrogen atoms at $10000\Delta t$, and (h) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface for the nitrogen atoms at $10000\Delta t$.

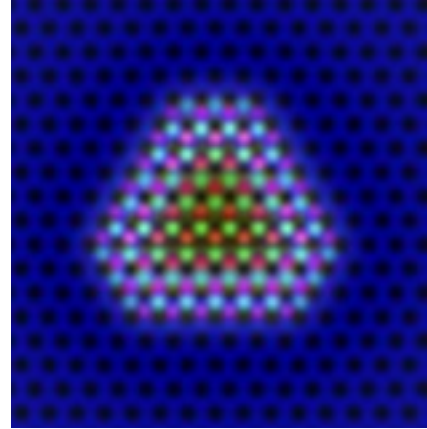
2. Multilayer jagged triangular crystals

Truncated triangular h-BN crystal, with multiple layers.

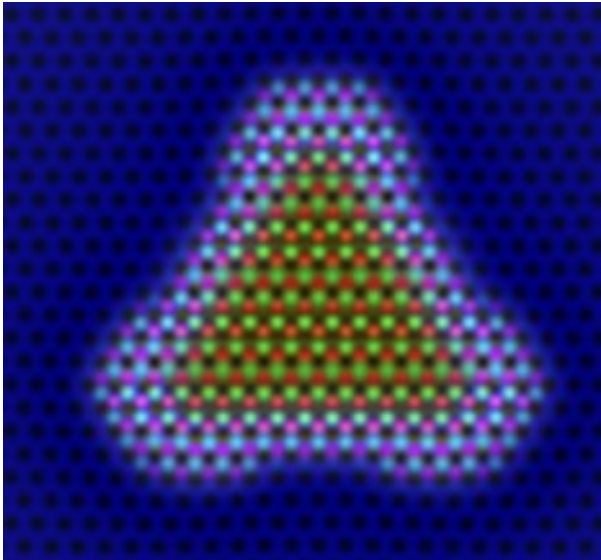
S.2.1. Example 1 with boron atoms on long edges and nitrogen atoms on short edges



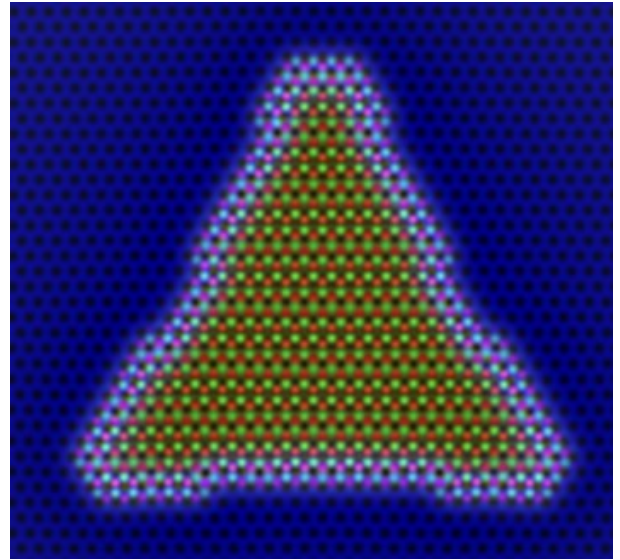
a.



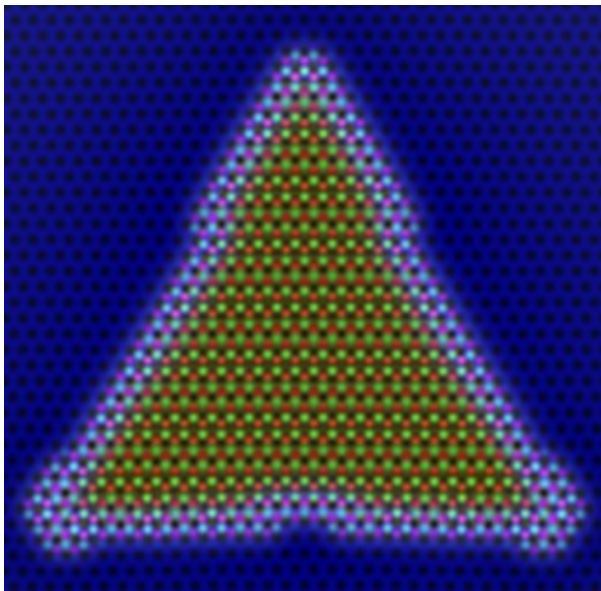
b.



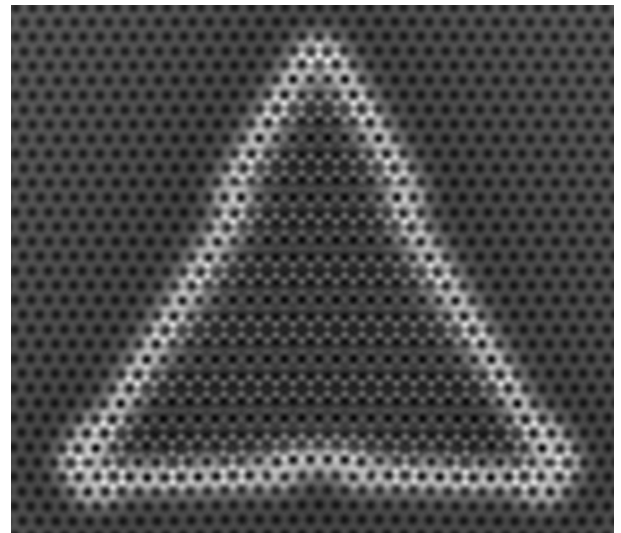
c.



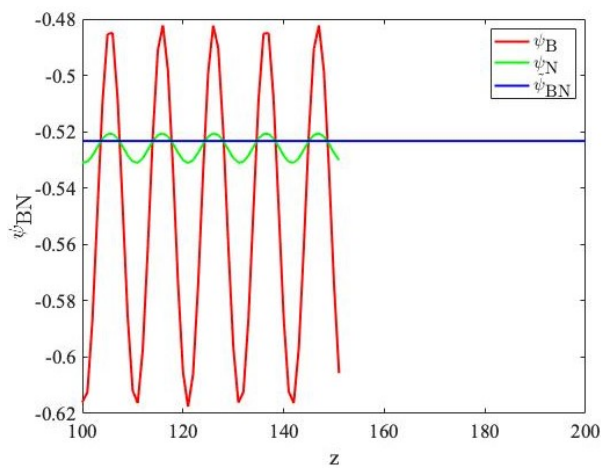
d.



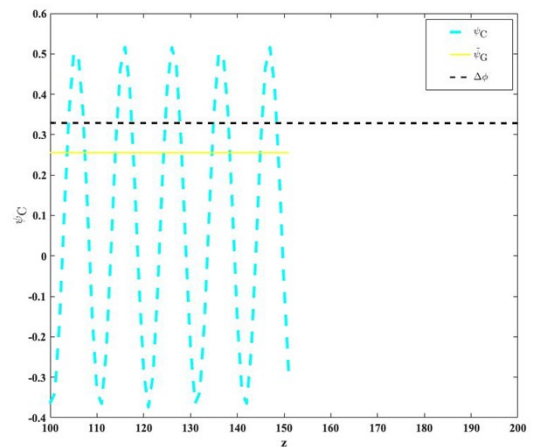
e.



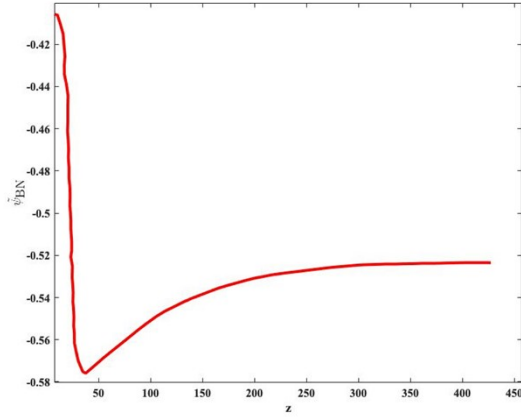
f.



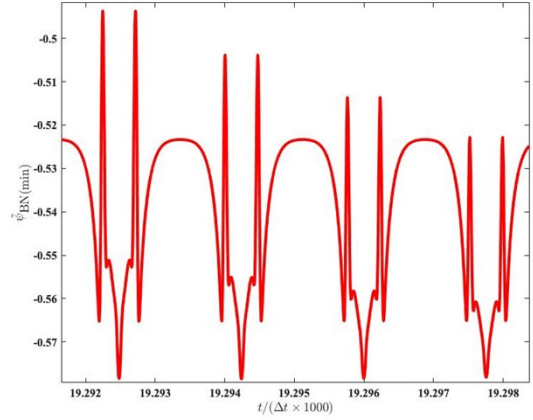
g.



h.



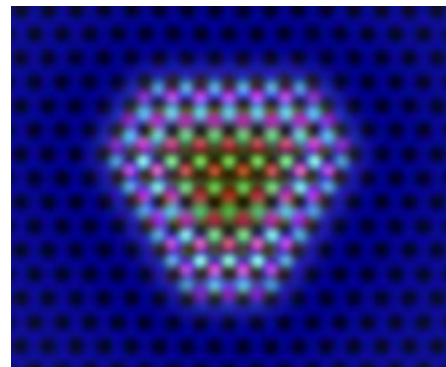
i.



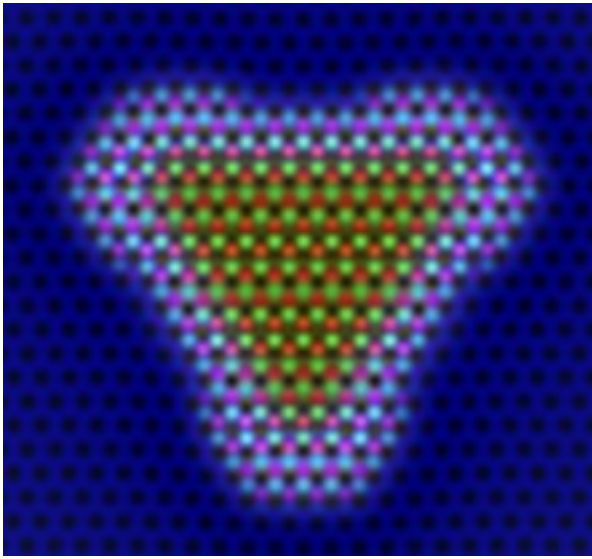
j.

FIG. S.2.1. (a) h-BN seed crystal placed at the center of the simulation box and is surrounded by graphene monolayer at $0\Delta t$, (b) a truncated hexagonal h-BN crystal is formed at $1000\Delta t$, (c) formation of additional layers around the corners of the truncated hexagonal h-BN crystal at $4000\Delta t$, (d) elongation of the truncated h-BN triangle and growth of multiple layers around the edges comprising of boron atoms of the truncated hexagonal h-BN crystal at $9000\Delta t$, (e) truncated h-BN triangle with multiple layers around the edges comprising of boron atoms formed at $10000\Delta t$. The short and long edges comprise of nitrogen and boron atoms, respectively, (f) density map of the crystal formed at $10000\Delta t$, (g) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front, (h) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where Z is the distance from the center of the particle, along the horizontal center line of the cluster, (i) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface at $10000\Delta t$, and (j) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface at $10000\Delta t$.

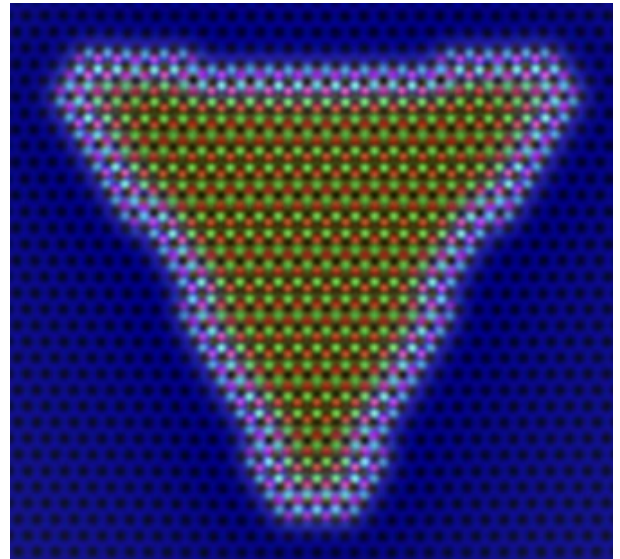
S.2.2 Example 1 with nitrogen atoms on long edges and boron atoms on short edges



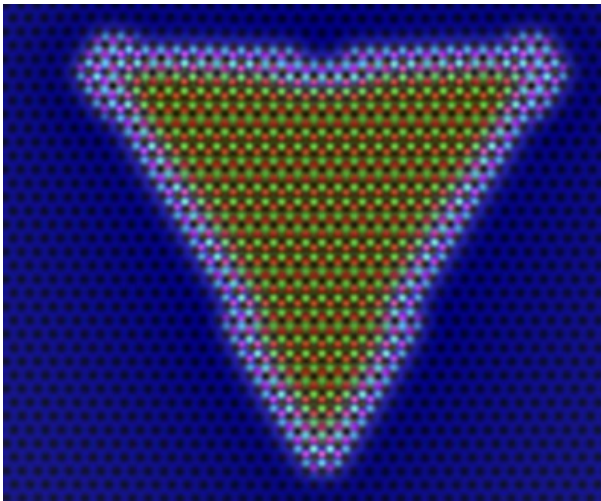
a.



b.



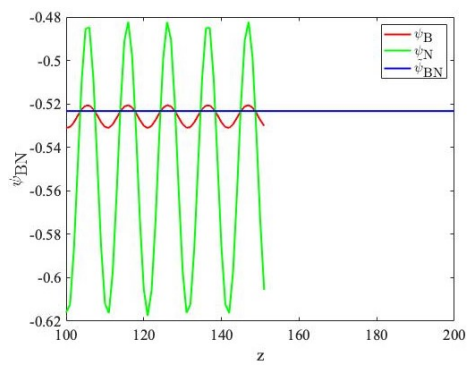
c.



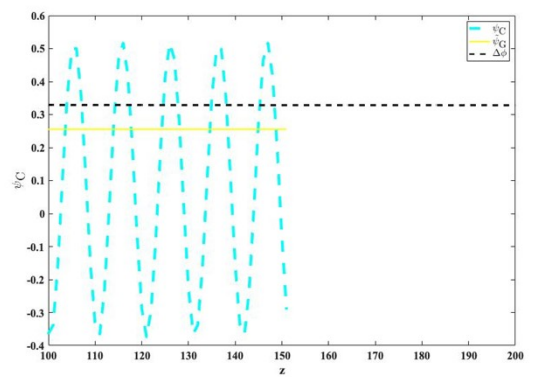
d.



e.

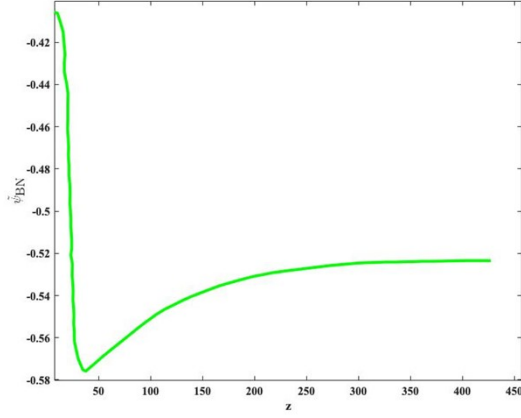


f.

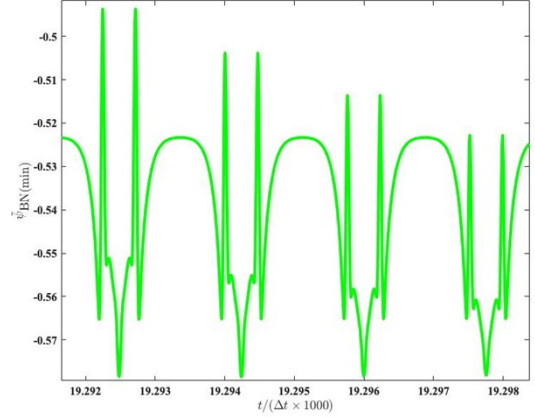


g.

h.



i.



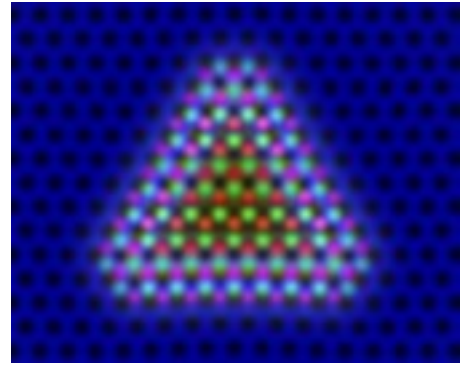
j.

FIG. S.2.2. (a) h-BN seed crystal placed at the center of the simulation box and is surrounded by graphene monolayer at $0\Delta t$, (b) a truncated hexagonal h-BN crystal is formed at $1000\Delta t$, (c) formation of additional layers around the corners of the truncated hexagonal h-BN crystal at $4000\Delta t$, (d) elongation of the truncated h-BN triangle and growth of multiple layers around the edges comprising of boron atoms of the truncated hexagonal h-BN crystal at $9000\Delta t$, (e) truncated h-BN triangle with multiple layers around the edges comprising of boron atoms formed at $10000\Delta t$. The short and long edges comprise of boron and nitrogen atoms, respectively, (f) density map of the crystal formed at $10000\Delta t$, (g) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front, (h) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where Z is the distance from the center of the particle, along the horizontal center line of the cluster, (i) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface at $10000\Delta t$, and (j) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface at $10000\Delta t$.

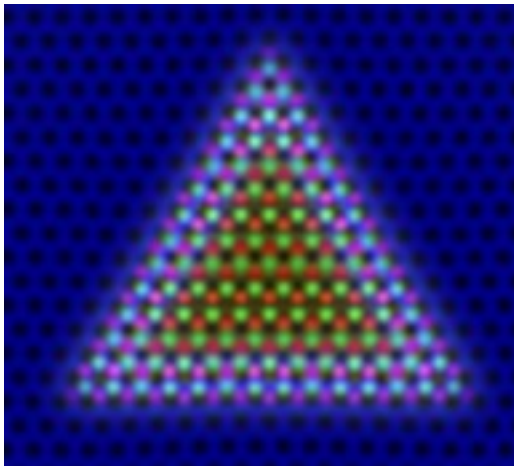
S.2.3 Example 2 with boron atoms on long edges and nitrogen atoms on short edges



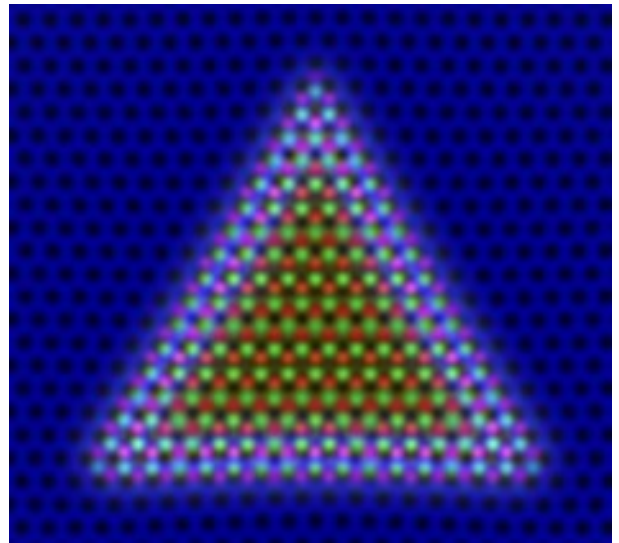
a.



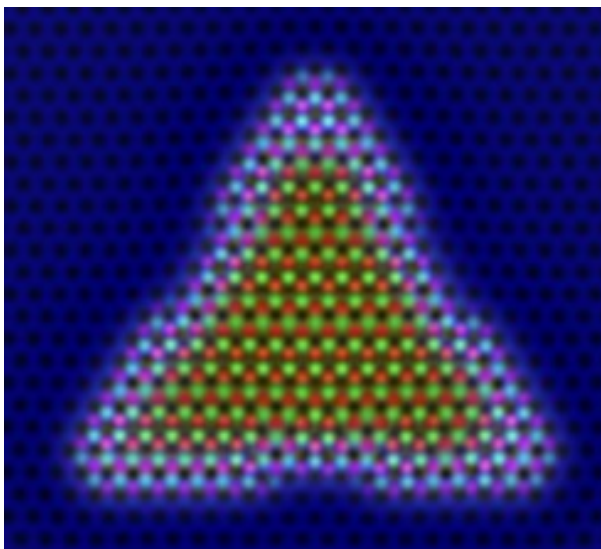
b.



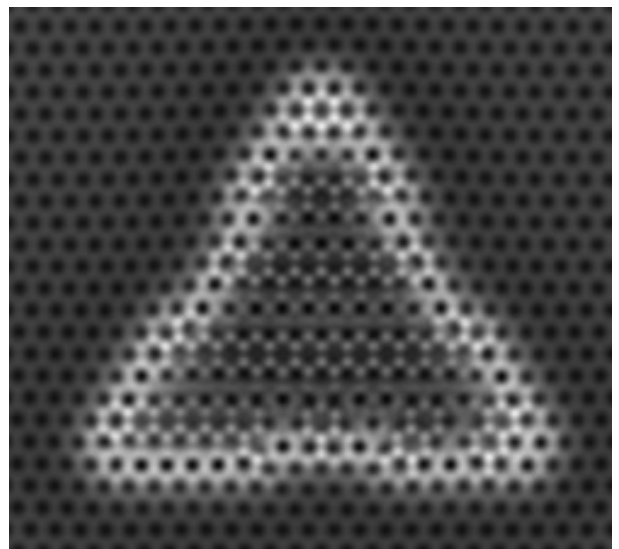
c.



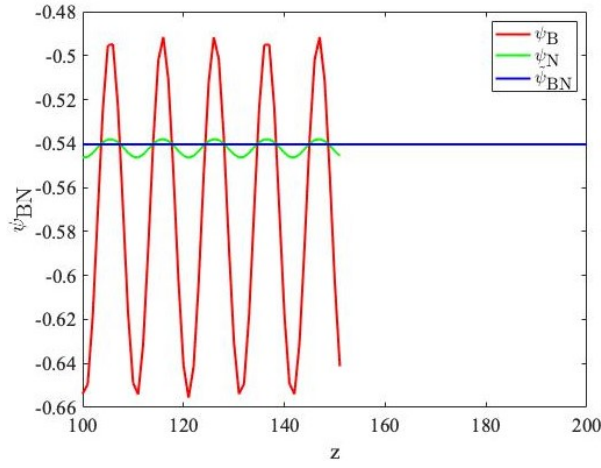
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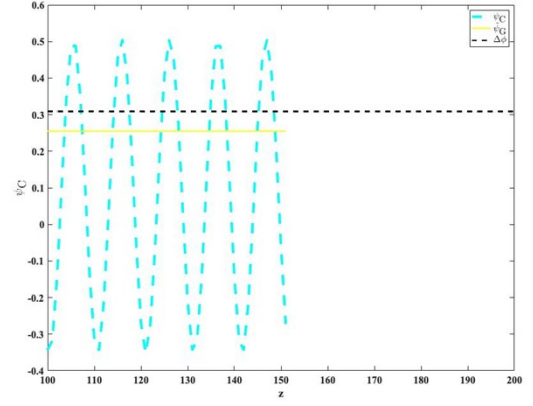
e.



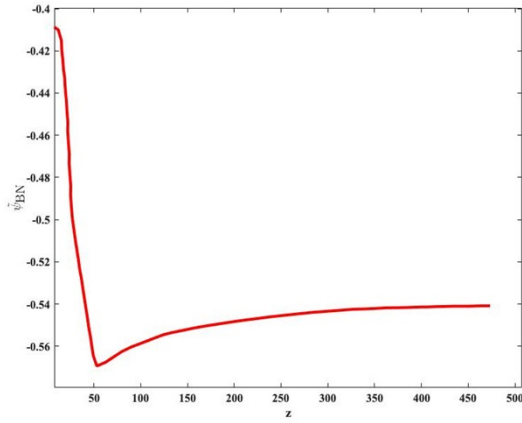
f.



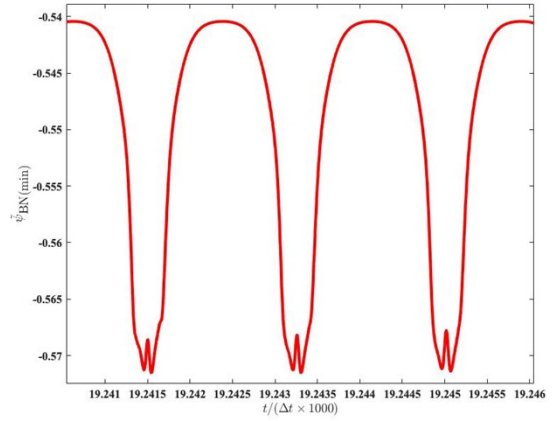
g.



h.



i.



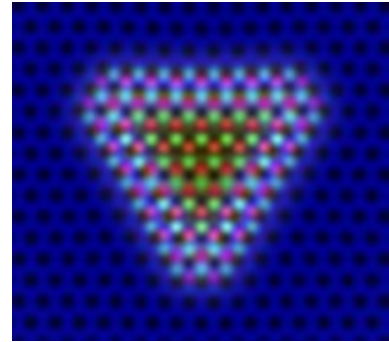
j.

FIG. S.2.3. (a) h-BN seed crystal placed at the center of the simulation box and is surrounded by graphene monolayer at $0\Delta t$, (b) formation of truncated hexagonal h-BN crystal at $3000\Delta t$, (c) growth of additional layers and formation of a triangular h-BN crystal at $6000\Delta t$, (d) increase in the size of h-BN crystal at $9000\Delta t$, (e) h-BN triangle with additional single layers formed at $10000\Delta t$. The short and long edges comprise of nitrogen and boron atoms, respectively, (f) density map of the crystal formed at $10000\Delta t$, (g) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front, (h) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (i) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface at $10000\Delta t$, and (j) the minimum density, $\psi_{BN(min)}$ of the liquid phase at $10000\Delta t$.

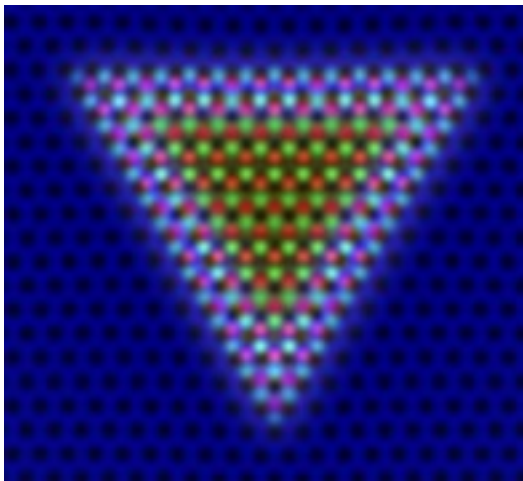
S.2.4 Example 2 with nitrogen atoms on long edges and boron atoms on short edges



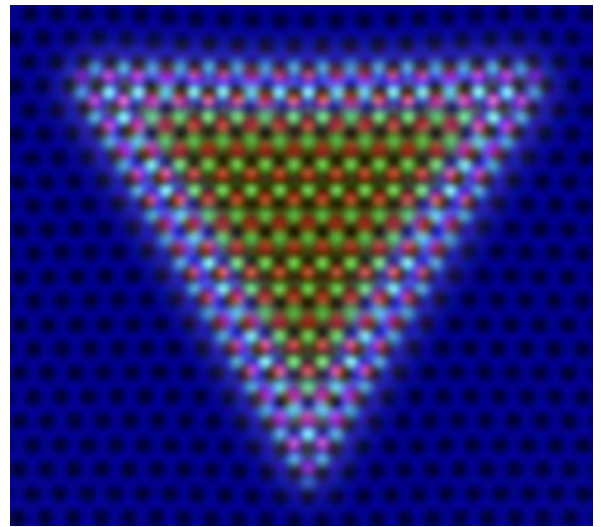
a.



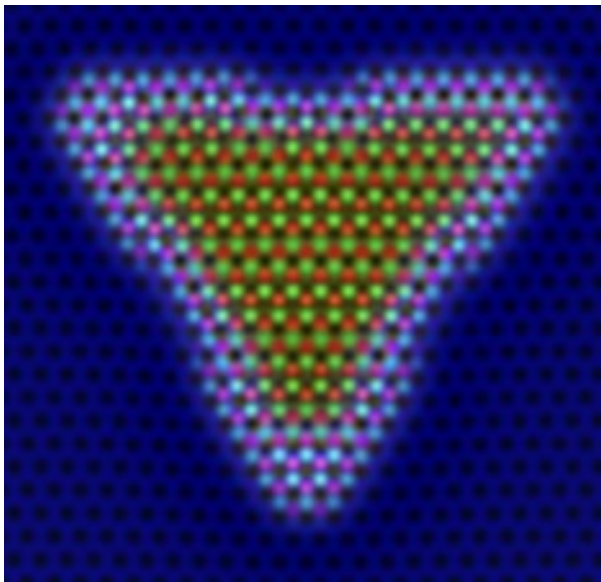
b.



c.



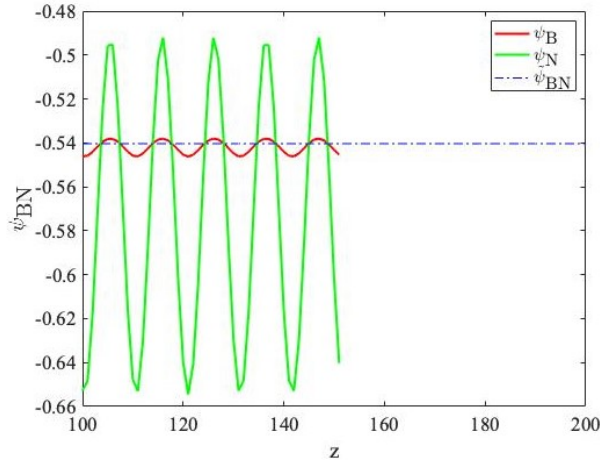
d.



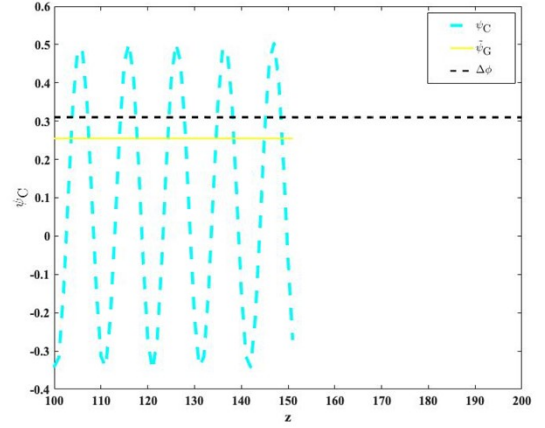
e.



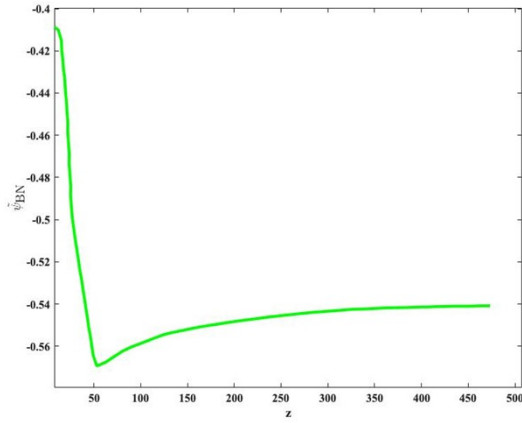
f.



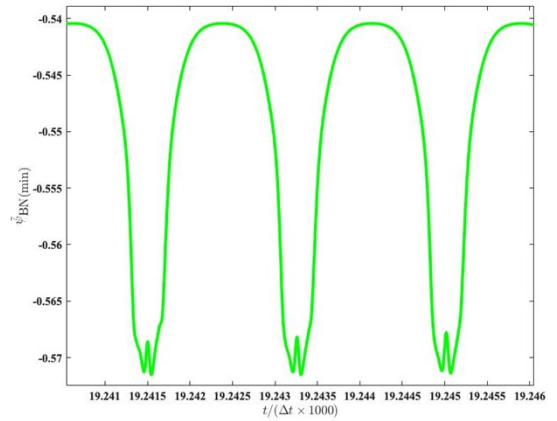
g.



h.



i.



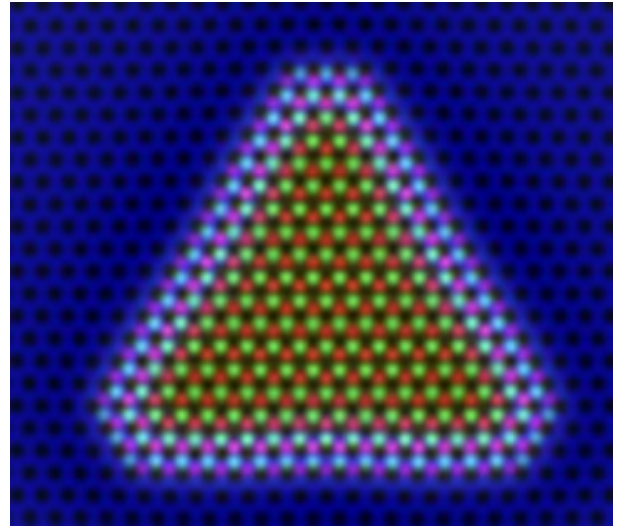
j.

FIG. S.2.4. (a) h-BN seed crystal placed at the center of the simulation box and is surrounded by graphene monolayer at $0\Delta t$, (b) formation of truncated hexagonal h-BN crystal at $3000\Delta t$, (c) growth of additional layers and formation of a triangular h-BN crystal at $6000\Delta t$, (d) increase in the size of h-BN crystal at $9000\Delta t$, (e) h-BN triangle with additional single layers formed at $10000\Delta t$. The short and long edges comprise of boron and nitrogen atoms, respectively, (f) density map of the crystal formed at $10000\Delta t$, (g) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front, (h) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (i) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface at $10000\Delta t$, and (j) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface at $10000\Delta t$.

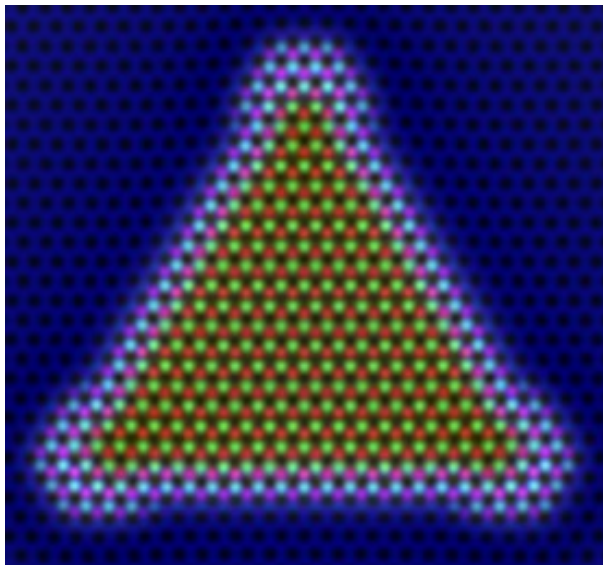
S. 2.5 Example 3 with boron atoms on long edges and nitrogen atoms on short edges



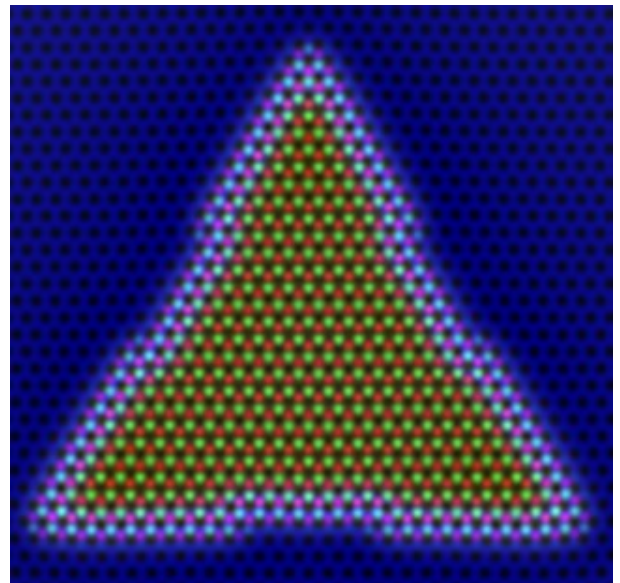
a.



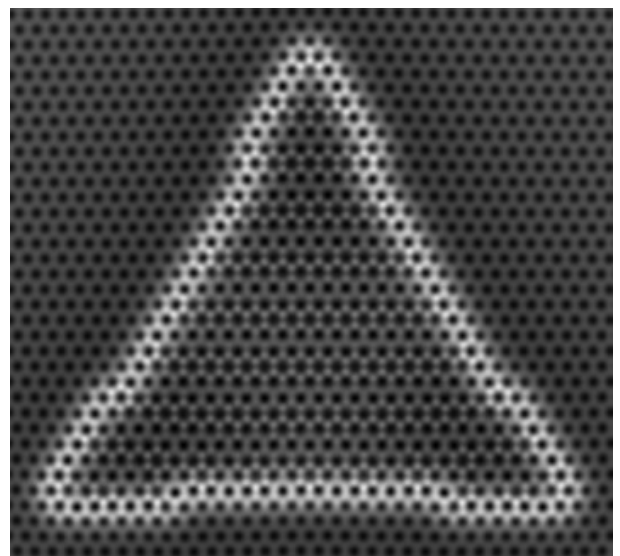
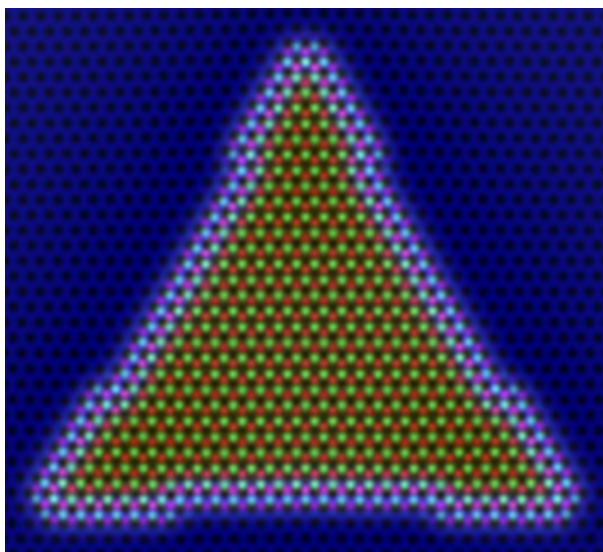
b.



c.



d.



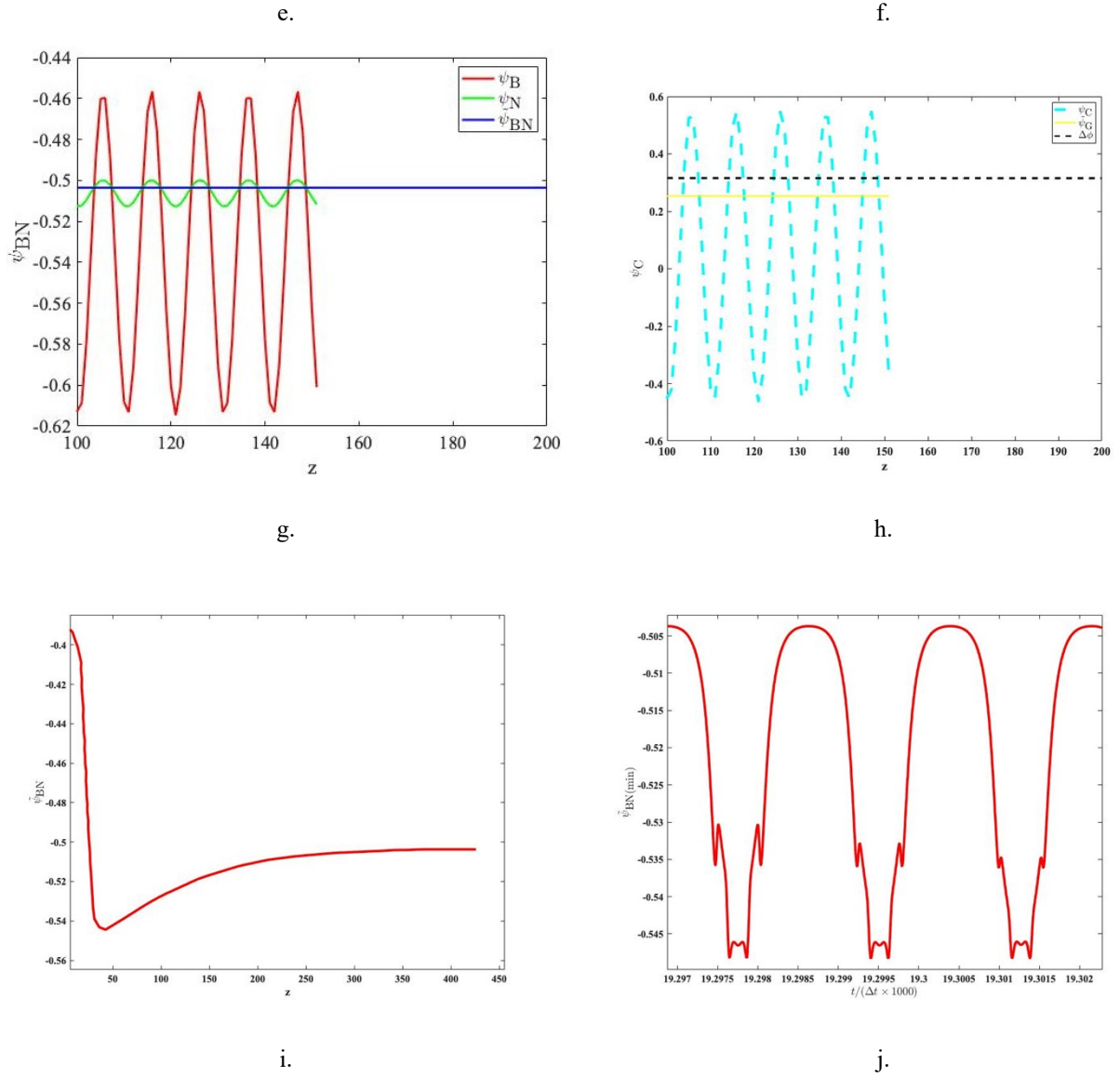
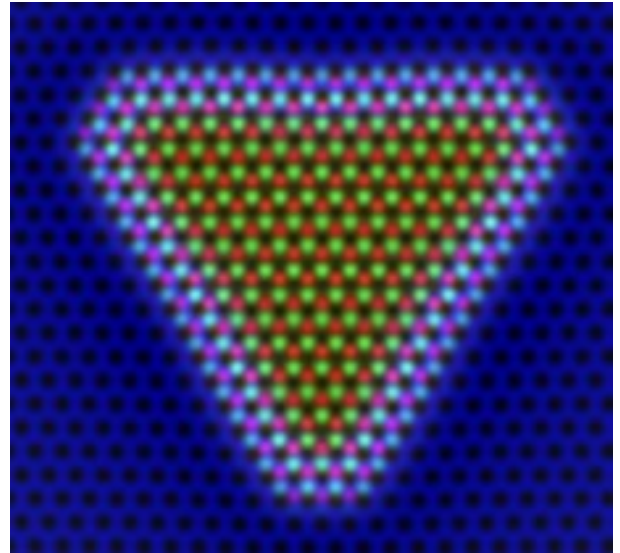


FIG. S.2.5 (a) h-BN seed crystal placed at the center of the simulation box and is surrounded by graphene monolayer at $0\Delta t$, (b) formation of truncated hexagonal h-BN crystal at $4000\Delta t$, (c) growth of additional layers and formation of a triangular h-BN crystal at $7000\Delta t$, (d) increase in the size of h-BN crystal at $9000\Delta t$, (e) h-BN triangle with additional single layers formed at $10000\Delta t$. The short and long edges comprise of nitrogen and boron atoms, respectively, (f) density map of the crystal formed at $10000\Delta t$, (g) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front, (h) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (i) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface at $10000\Delta t$, and (j) the minimum density, $\psi_{BN}^{(min)}$ of the liquid phase on front of solid-liquid interface at $10000\Delta t$.

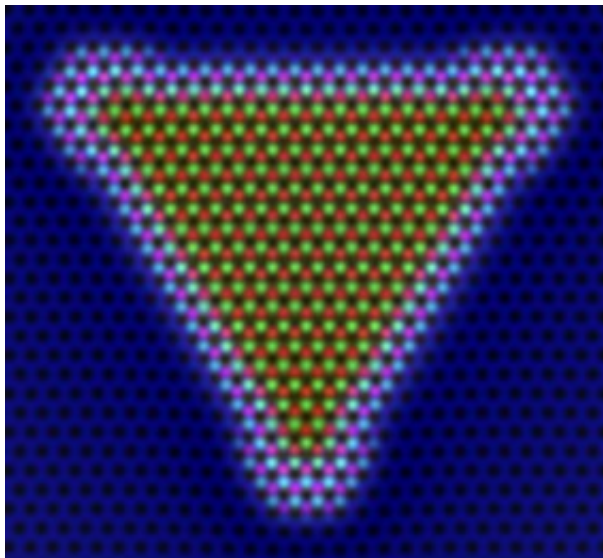
S.2.6 Example 3 with nitrogen atoms on long edges and boron atoms on short edges



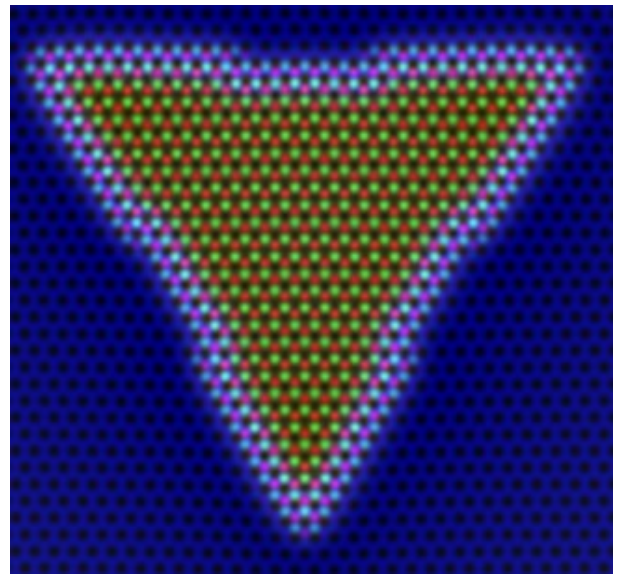
a.



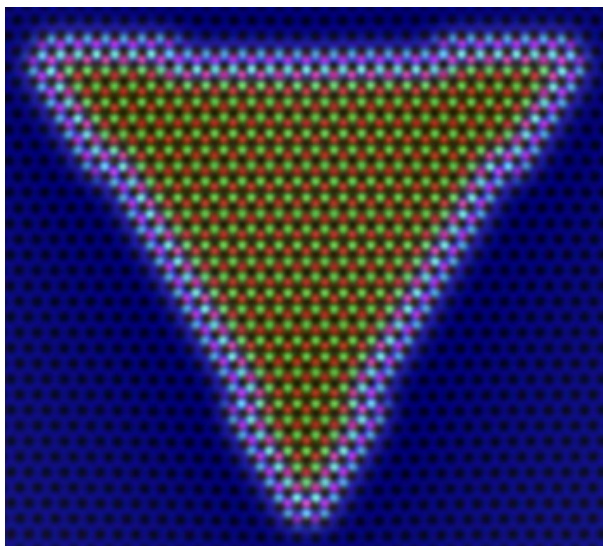
b.



c.



d.



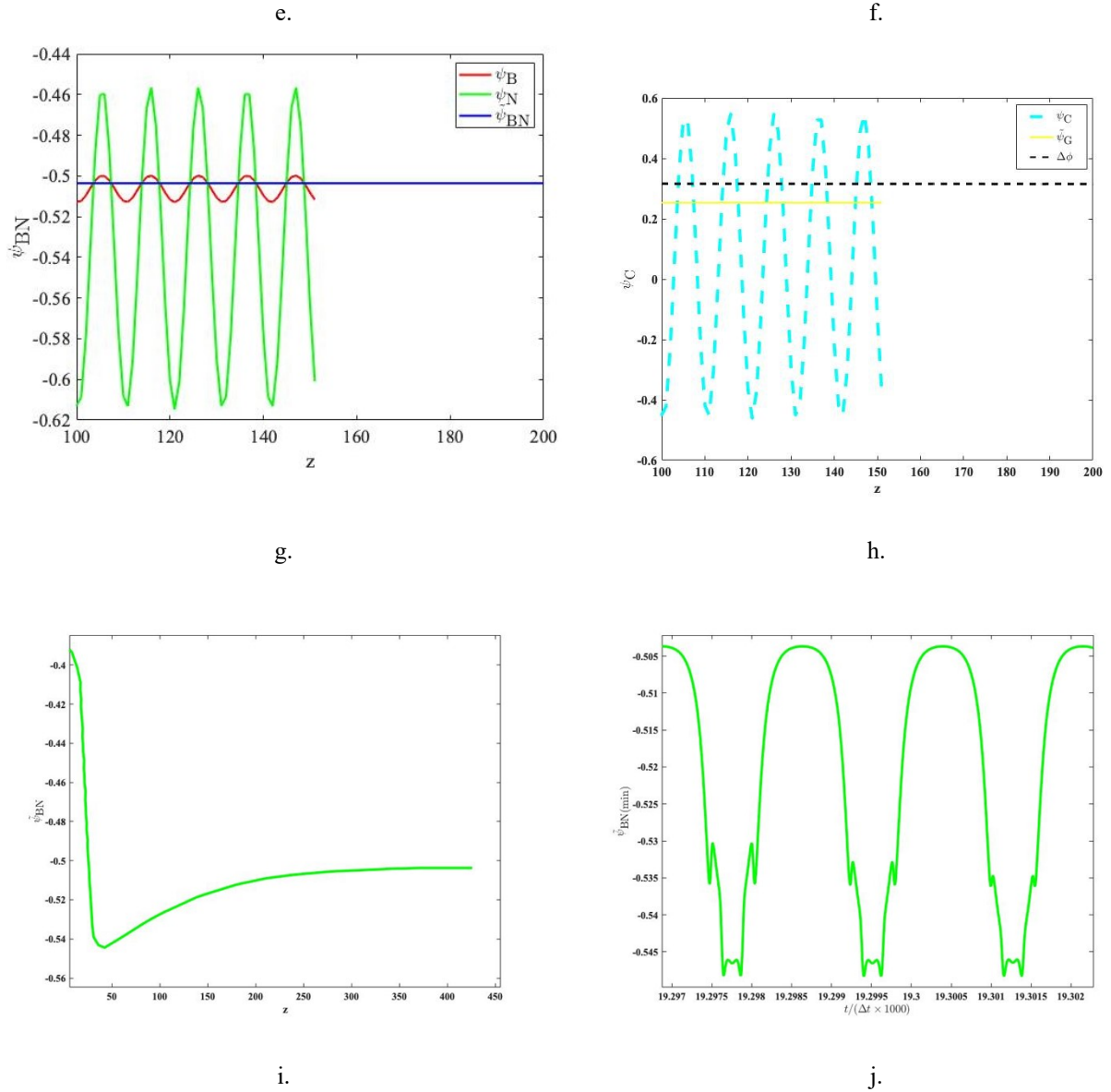


FIG. S. 2.6. (a) h-BN seed crystal placed at the center of the simulation box and is surrounded by graphene monolayer at $0\Delta t$, (b) formation of truncated hexagonal h-BN crystal at $4000\Delta t$, (c) growth of additional layers and formation of a triangular h-BN crystal at $7000\Delta t$, (d) increase in the size of h-BN crystal at $9000\Delta t$, (e) h-BN triangle with additional single layers formed at $10000\Delta t$. The short and long edges comprise of boron and nitrogen atoms, respectively, (f) density map of the crystal formed at $10000\Delta t$, (g) the local particle density for boron, ψ_B and nitrogen ψ_N particles, and average particle density, ψ_{BN} at the growth front, (h) the local particle density for carbon, ψ_C particle, and average particle density of graphene, ψ_G at the growth front, where z is the distance from the center of the particle, along the horizontal center line of the cluster, (i) shape of the smoothed density profile, ψ_{BN} on the front of solid-liquid interface at $10000\Delta t$, and (j) the minimum density, $\psi_{BN(min)}$ of the liquid phase on front of solid-liquid interface at $10000\Delta t$.