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Supplementary Information for Stable, One-Dimensional Suspended and Supported Monatomic Chains of Pnictogens: A Metal-Insulator Framework

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1 Supported zigzag monatomic chains of pnictogens

Further to the results presented in Sec. IV-A (Zigzag chains supported by substrates) of the paper, here we present additional results about zigzag pnictogen chains (As-*ZZ*, Sb-*ZZ*, Bi-*ZZ*) supported by their parent 2D monolayers (arsenene, antimonene, bismuthene, respectively), as well as P-*ZZ* on graphene and GaSe monolayers. In the following figures we present top and side views of atomic configurations obtained by the full optimization of structures; top and side views of the snapshots taken in AIMD calculations performed at T=300 K for 4 ps; total density of states (TDOS) together with local density of states (LDOS) at the supported chain and energy band structure around the band gap. Our analysis shows that the zigzag monatomic chains are bound weakly with the underlying substrates. Accordingly, they are held at a large distance from the surface of substrate. Supported chains are stable, and preserve electronic properties when they were free-standing.

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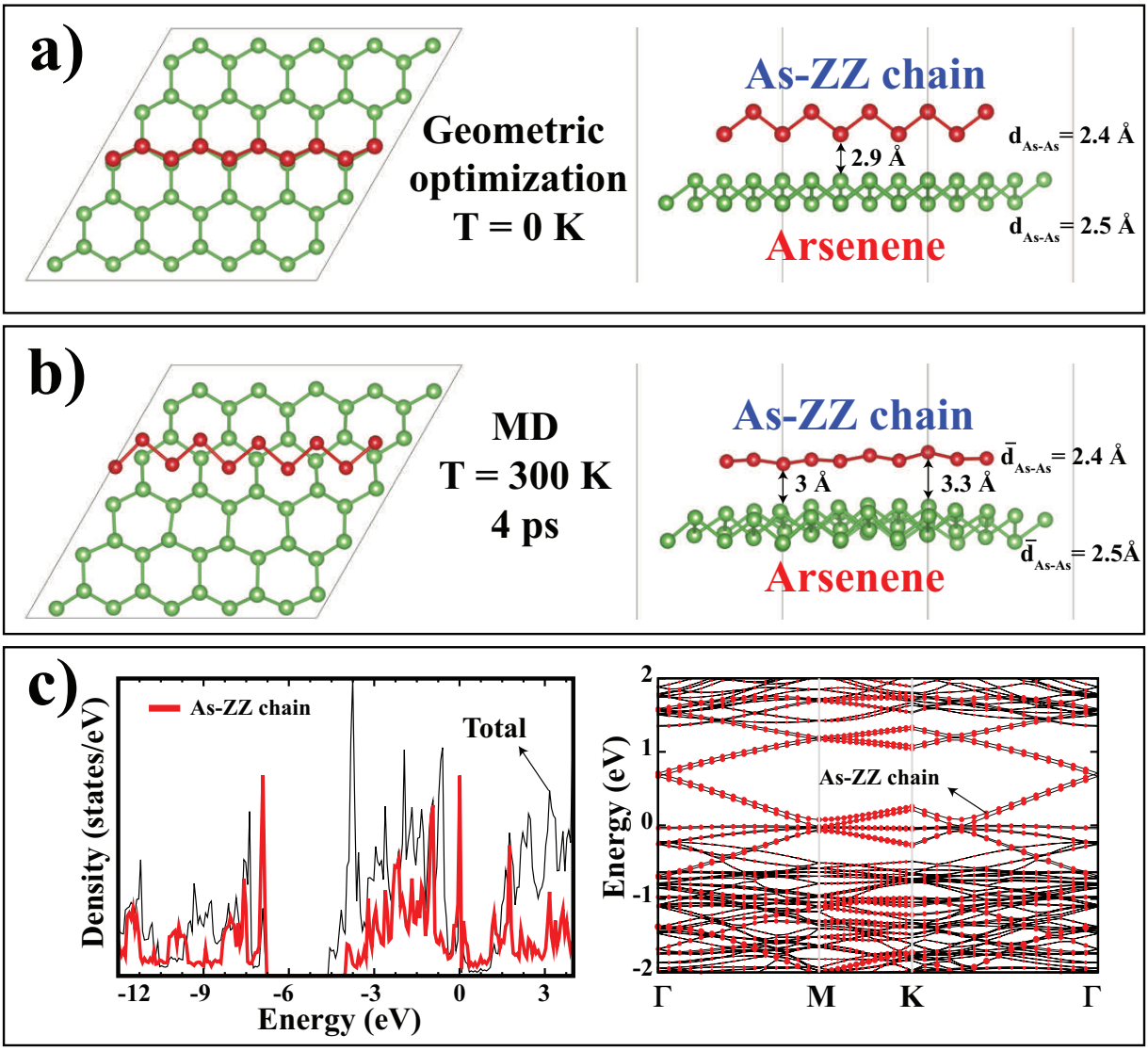

Fig. S1 (Color online) (a) Top side and side view of optimized As-ZZ chain + arsenene substrate. (b) Top and side view of the snapshots taken from *ab initio* molecular dynamic, AIMD calculations performed at T=300 K for 4 ps. (c) Total density of states (TDOS) together with the local density of states (LDOS) at the supported chain and electronic band structure of optimized As-ZZ chain + arsenene substrate, As-ZZ chain contribution indicated using red line and circles, DOS of As-ZZ chain multiplied by six. The Fermi level is set to the zero energy.

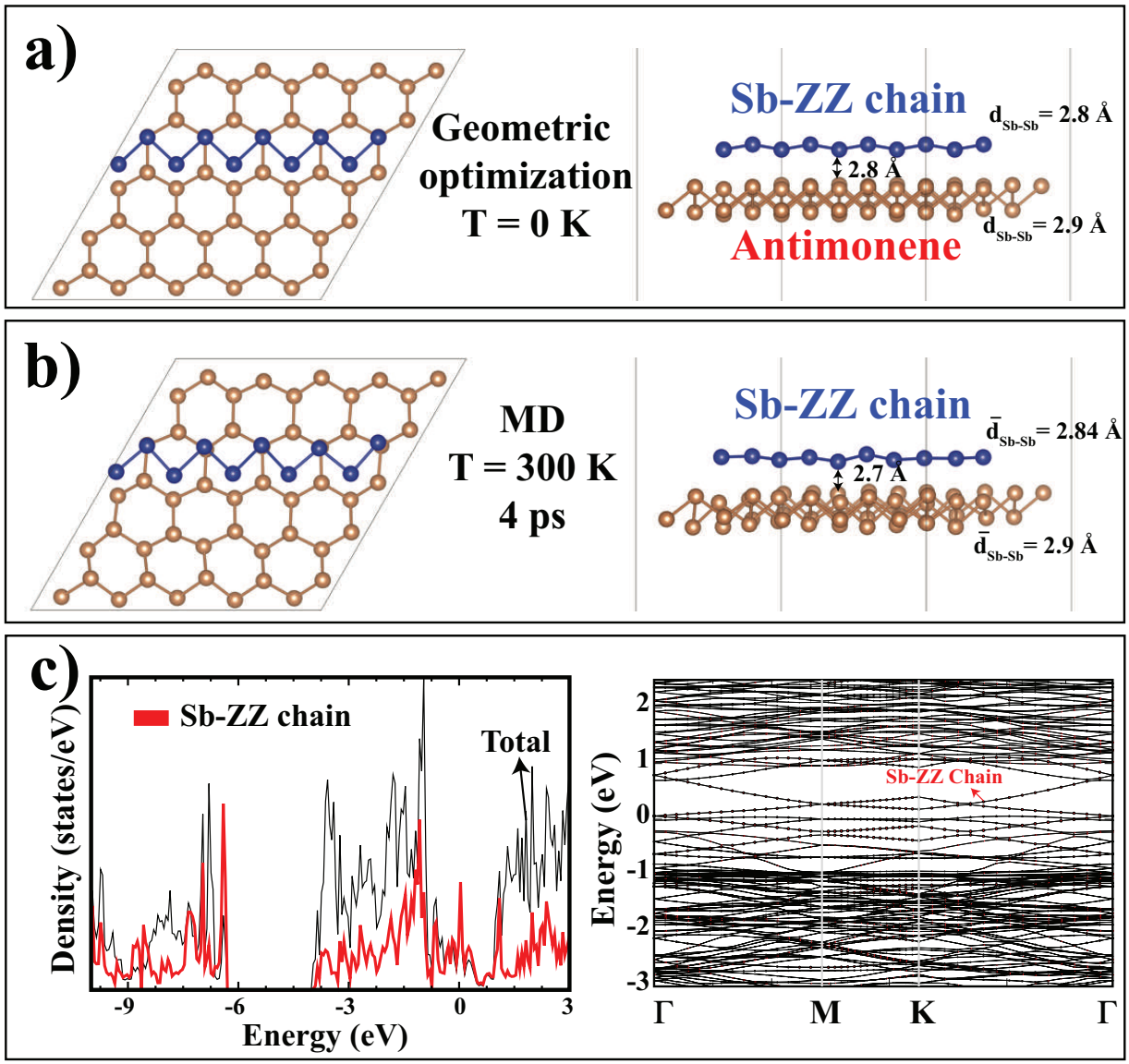

Fig. S2 (Color online) a) Top and side view of optimized Sb-ZZ chain + antimonene substrate. b) Top and side view of snapshots taken from *ab initio* molecular dynamic AIMD simulations performed at T=300K for 4ps. (c) Total density of states (TDOS) together with the local density of states at the supported chain and electronic band structure of optimized Sb-ZZ chain + antimonene substrate, Sb-ZZ chain contribution indicated using red line and circles, DOS of Sb-ZZ chain multiplied by six.The Fermi level is set to the zero energy.

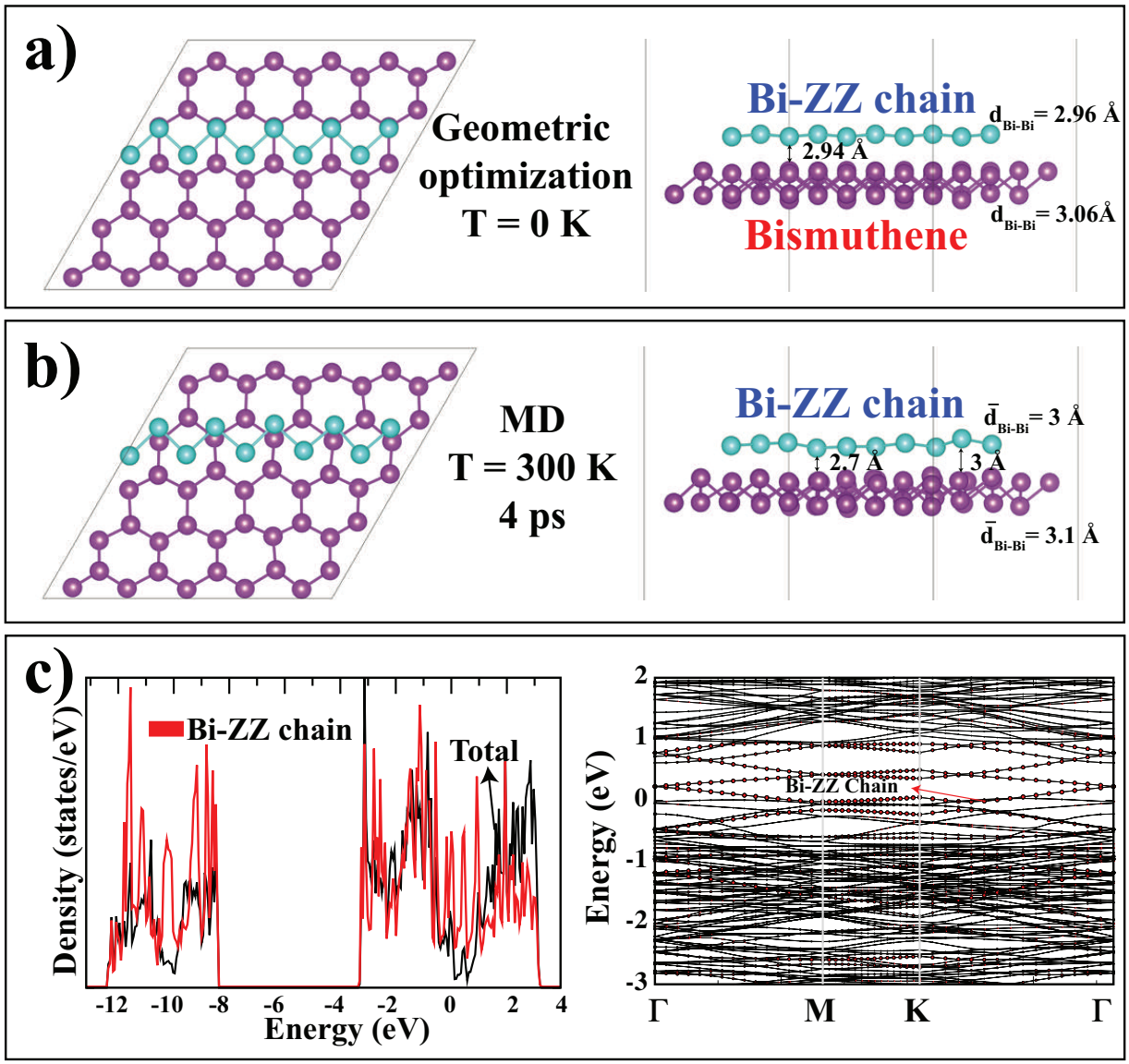

Fig. S3 (Color online) a) Top and side view of optimized Bi-ZZ chain + bismuthene substrate. (b) Top and side view of the snapshots taken from *ab initio* molecular dynamic (MD) simulation performed at T=300 K for 4 ps. (c) Total density of states (DOS) and together with the local density of states (LDOS) at the supported P-*ZZ* chain and electronic band structure of optimized Bi-ZZ chain + bismuthene substrate, Bi-ZZ chain contribution indicated using red line and circles, DOS of Bi-ZZ chain multiplied by six.The Fermi level is set to the zero energy.

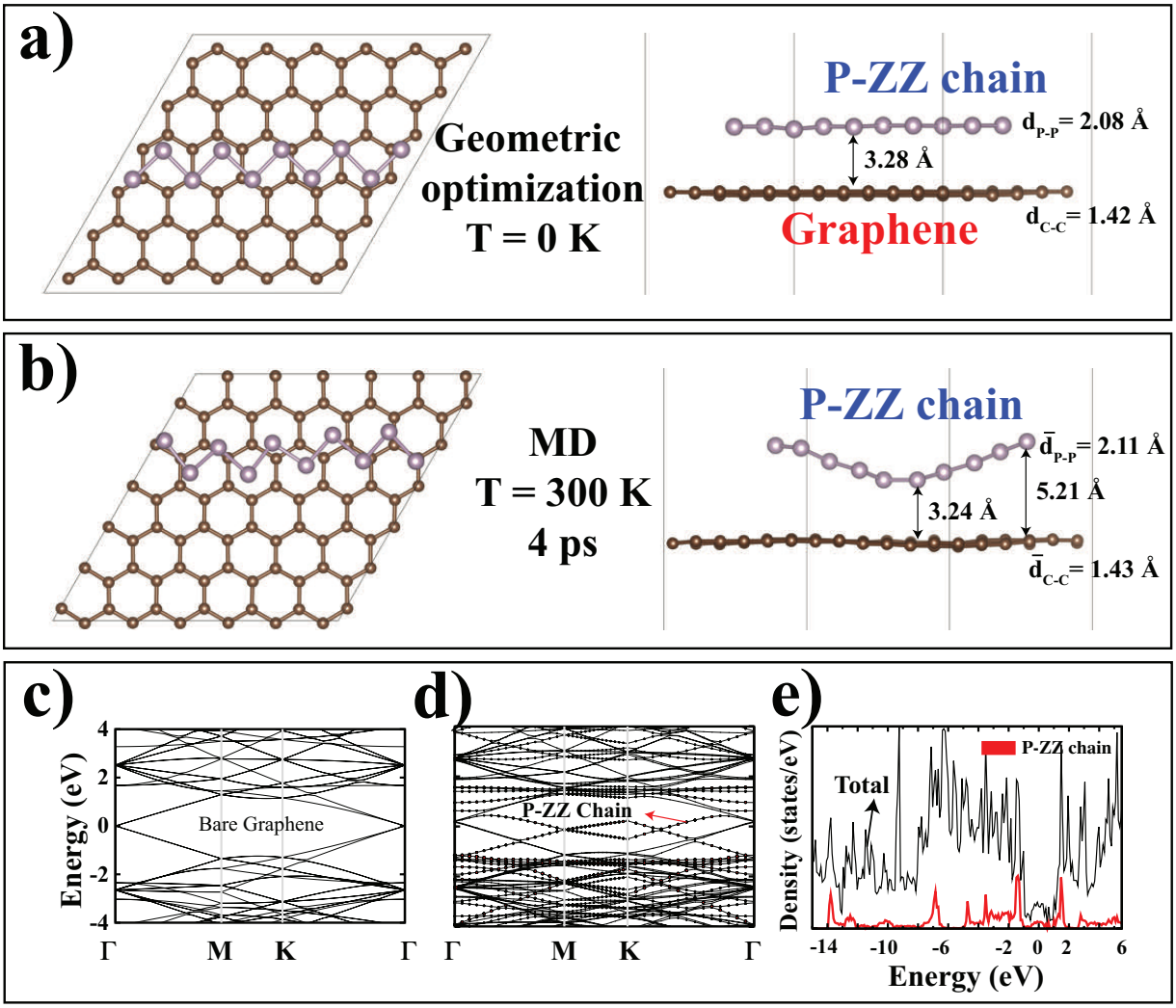

Fig. S4 (Color online) a) Top and side views of optimized P-*ZZ* chain + graphene substrate. (b) Top and side view of the snapshots taken from *ab initio* molecular dynamic (AIMD) simulations performed at T=300 K at 4 ps. (c) Electronic band structure of bare graphene (6×6 supercell). (d)and (e) Electronic band structure and total (DOS) together with the local density of states (LDOS) at the supported chain calculated for the optimized P-*ZZ* chain + graphene substrate, P-*ZZ* chain contribution indicated using red line and circles.The Fermi level is set to the zero energy.

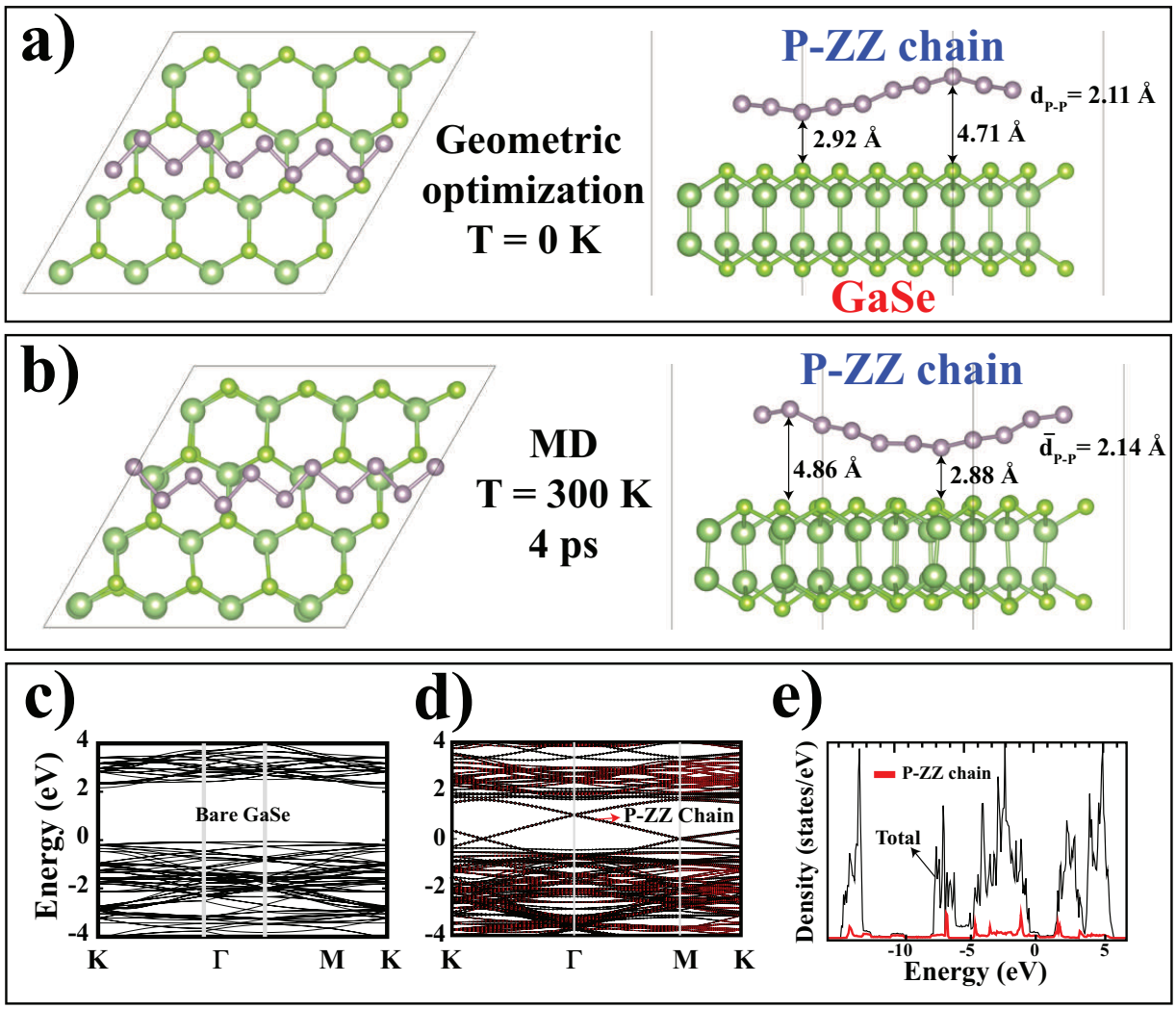

Fig. S5 (Color online) (a) Top and side views of optimized P-*ZZ* chain + GaSe substrate. (b) Top and side views of the snapshots taken from *ab initio* molecular dynamic AIMD simulations performed at T=300 K and 4ps. (c) electronic band structure of bare GaSe (4×4 supercell), d),e) electronic band structure and density of states (DOS) of optimized (T=0K) P-ZZ chain + GaSe substrate, P-ZZ chain contribution indicated using red line and circles.The Fermi level is set to the zero energy.