Electronic Supplementary Material (ESI) for RSC Advances.

First-principles study of Indium nitride monolayer doped with alkaline earth metals

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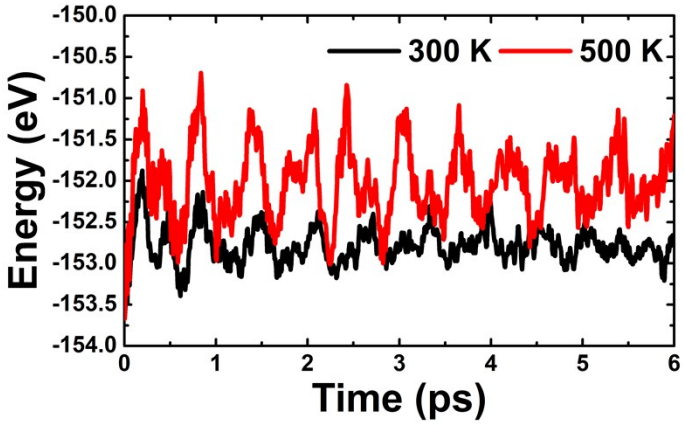

Figure S1. AIMD simulation at 300and 500K of InN monolayer.

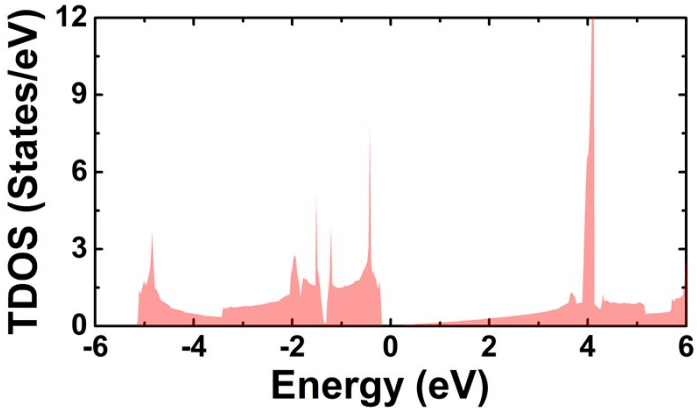

Figure S2: Total density of states of InN monolayer.

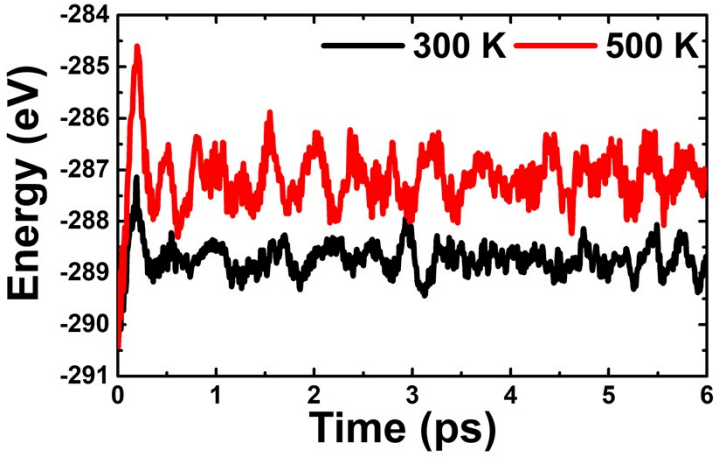

Figure S3: AIMD simulations at 300and 500K of InN monolayer with a single In vacancy.

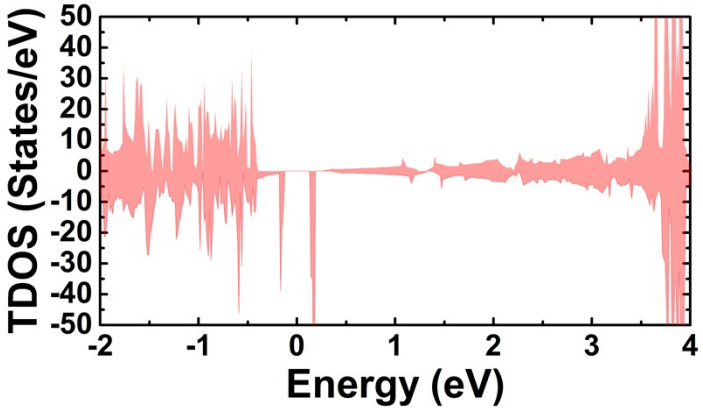

Figure S4: Total density of states of InN monolayer with a single In vacancy.

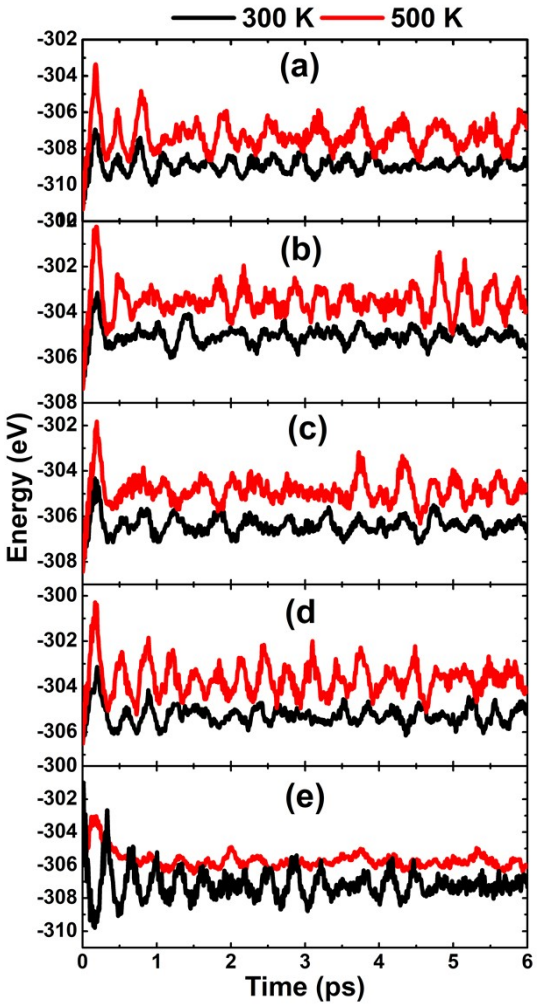

Figure S5: AIMD simulations at 300 and 500K of InN monolayer doped with (a) Be, (b) Mg, (c) Ca, (d) Sr, and (e) Ba.

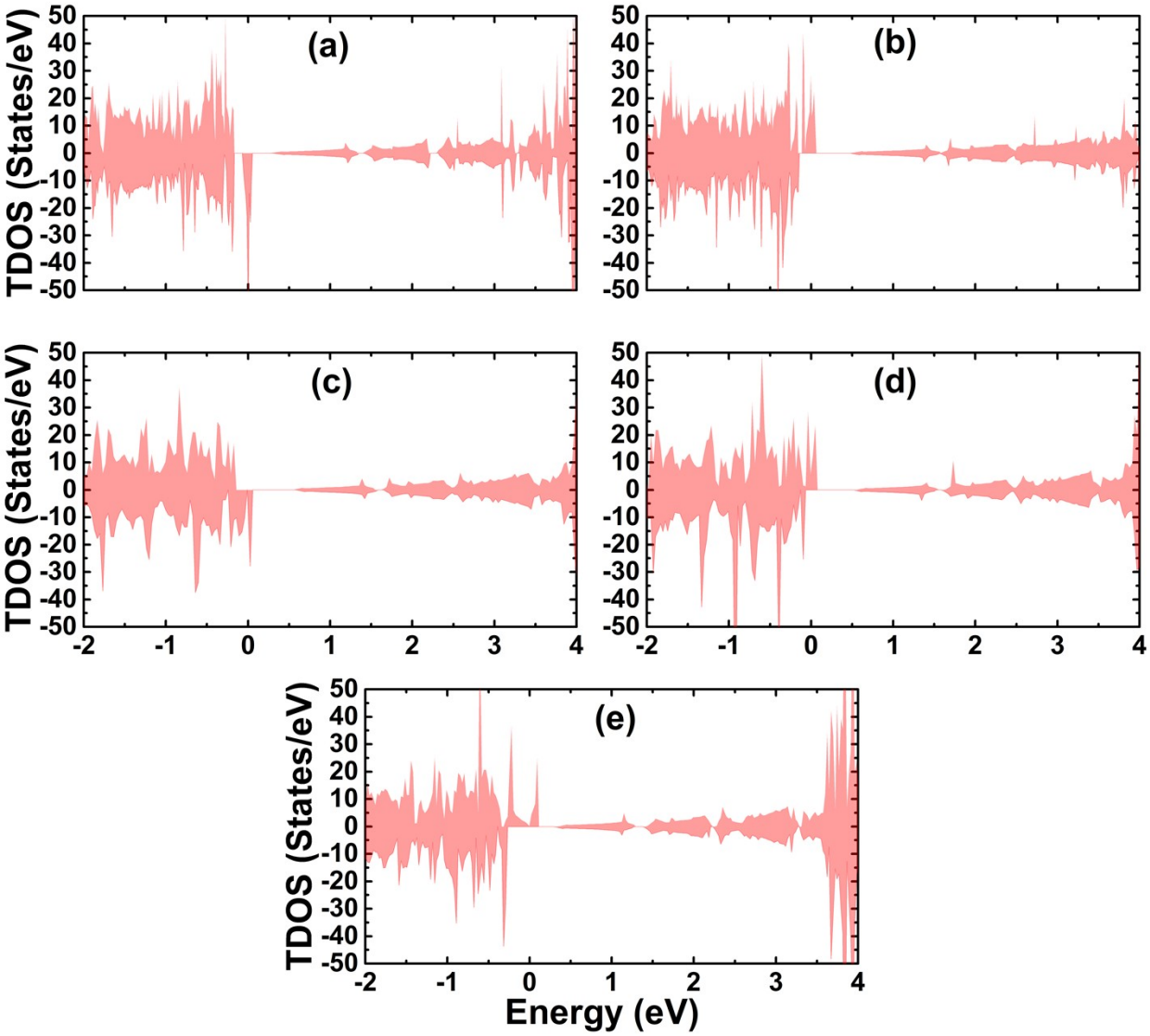

Figure S6: Total density of states of InN monolayer doped with (a) Be, (b) Mg, (c) Ca, (d) Sr, and (e) Ba.

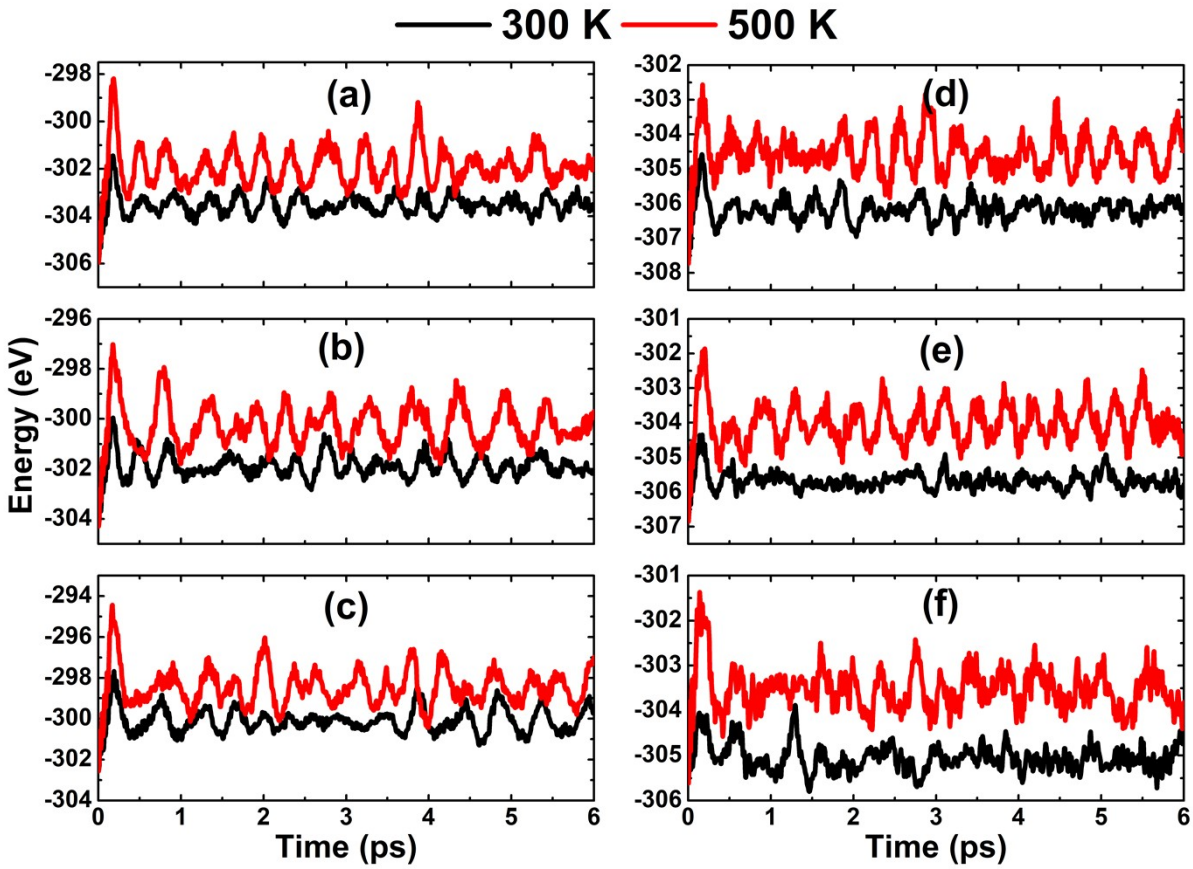

Figure S7: AIMD simulations at 300and 500K of InN monolayer doped with (a) 12.5%, (b) 18.75%, (c) 25% of Mg; and (d) 12.5%, (e) 18.75%, and (f) 25% of Ca.