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Next Generation Monolayer Structures of Group V Elements: Nitrogene and Antimonene ONGUN OZCELIK, Princeton University, OLCAY AKTURK, ENGIN DURGUN, SALIM CIRACI, Bilkent University — Based on first-principles density functional theory, we predict that nitrogen and antimony atoms can form single-layer, buckled honeycomb structures called nitrogene[1] and antimonene[2], which are rigid and stable even above room temperature. The 2D crystalline phase of nitrogen, which corresponds to a local minimum in the Born-Oppenheimer surface, is a nonmagnetic insulator with saturated pi bonds. When grown on a substrate like Al(111) surface or graphene, nitrogene binds weakly to substrates and hence preserves its free-standing properties, but it can easily be pealed off. Zigzag and armchair nanoribbons have fundamental band gaps derived from reconstructed edge states. These band gaps are tunable with size and suitable for the emerging field of 2D electronics. Nitrogene and antimonene form not only bilayer, but also 3D graphitic multilayer structures. Single-layer nitrogene can nucleate and grow on the armchair edges of hexagonal boron nitride. Starting from the pseudo-layered character of 3D bulk crystals of antimony, we also demonstrate the formation of monolayer antimonene structure which is similar to nitrogene. [1] Phys. Rev. B 92, 125420, 2015. [2] Phys. Rev. B 91, 235446, 2015.

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