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Novel Electronic Properties of Si-Doped Boron Nitride Monolayers SANJEEV GUPTA, Department of Physics, Michigan Technological University, Houghton, Michigan 49931, USA, HAIYING HE, Department of Physics and Astronomy, Valparaiso University, Valparaiso, IN 46383, USA, DOUGLAS BANYAI, MINGSU SI[1], RAVINDRA PANDEY, Department of Physics, Michigan Technological University, Houghton, Michigan 49931, USA, SHASHI KARNA, US Army Research Laboratory, Weapons and Materials Research Directorate, ATTN: RDRL-WM, Aberdeen Proving Ground, MD 21005-5069, USA — In this work, we address the most critical fundamental question on the effect of doping, especially by Si, on the stability, electronic, magnetic and electron transport properties of the two-dimensional BN monolayers using density functional theory. Si substitutions at B, N and a divacancy site created by the removal of a B-N pair are investigated. The non-equal valence state of the Si dopant leads to a non-zero magnetic moment for the single site substitution. Si-induced gap states in BN monolayer energy spectrum are also observed, which demonstrate profound impact on the electron transport properties of the BN monolayer. Unique features in the device characteristics of Si-doped BN monolayers are predicted including a significant enhancement of current at the Si site, diode-like asymmetric current-voltage response and negative differential resistance. The calculated STM images clearly discern the site-dependence of Si dopants in the monolayer.

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