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Strain Engineering of Phosphorene via Bending DEEPTI VERMA, Department of Chemical Engineering and Materials Science, University of Minnesota, TRAIAN DUMITRICA, Department of Mechanical Engineering, University of Minnesota — Phosphorene (PE) - the newly discovered 2D derivative of Phosphorus - has an inherent band gap and a high current on/off ratio. Manipulating strain in PE films - strain engineering (SE) - will offer the opportunity to further tailor its electronic properties. Using objective boundary conditions (OBC) coupled with density functional tight binding model (DFTB), we calculate bending rigidity of PE and its 2D allotropes by modeling bent PE as large diameter nanotubes (PNTs). OBCs not only allow for drastic reductions in the number of atoms in simulations but also enable simulations of chiral PNTs, which is impossible with periodic boundary conditions. At the same time, the method describes how bending influences the electronic structure. We establish a robust platform for achieving SE for anisotropic 2D films. Using results from our calculations and orthotropic thin shell model we develop equivalent continuum structure (ECS) for PE and its allotropes upon bending. The developed ECS can be used for performing finite element simulations of PE films on substrates.

Deepti Verma
Department of Chemical Engineering and Materials Science, University of Minnesota

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