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Chemi- and physisorption of hydrogen on graphitic substrates
BORIS YAKOBSON, ABHISHEK SINGH, JIANXIN LU, MORGANA RIBAS, Department of Mechanical Engineering and Materials Science, Rice University, Houston, TX 77006 — We evaluate the possibilities of hydrogen storage on graphitic substrates by chemical and physical sorption using multiscale modeling. Detailed thermodynamic analysis based on ab initio calculations of chemisorptions via catalytic spillover shows that the catalyst saturation and improved C-H binding energies are the key to enhanced storage [1]. The estimation of amount of physisorbed hydrogen under the ambient condition in 3D-foams using grand canonical Monte Carlo simulations demands judicious choice of interaction potential and incorporation of quantum corrections due to large thermal de Brogile wavelength. We will show that the storage capacities (chemi- or physisorption) in graphitic materials can meet the DOE 2015 targets.

[1] A. K. Singh, M. A. Ribas, and Boris I. Yakobson, ACS Nano, 3, 1657 (2009).

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