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Titanium Doped Carbon Nanotubes for Hydrogen Storage JAKE FENNICK, JAMES LEWIS, West Virginia University — An efficient method of storing hydrogen is necessary before fuel cells can become practical. Previous computational results show that a single titanium atom adsorbed on the surface of a carbon nanotube can bind up to 4 hydrogen molecules. We pursue simulations of hydrogen packed between two titanium-doped carbon nanotubes. The highest percentage weight of storage and the manner in which these parallel nanotubes pack is of particular interest. Calculations are performed with the classical MD program GULP. After computation, automated analysis will choose the combination of parameters that results in the most efficient hydrogen storage for these titanium-doped carbon nanotube systems.
[1] Yildrim, T.; Ciraci, S. Phys. ReV. Lett. 2005, 94, 175501.

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