

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

The Titanium-Boron Nitride interaction GERARDO J. VAZQUEZ, FERNANDO MAGANA, EDUARDO RANGEL, GREGORIO RUIZ, Instituto de Fisica — The Boron Nitride (BN) has a structure very similar to that of graphite and this what makes it interesting to study. A sheet of BN has a structure similar to that of the graphene. In this work it was studied, using molecular dynamics based on pseudopotentials theory and Density Functional Theory (DFT), the energy of interaction of a titanium atom with a sheet of BN to obtain the position of adsorption of the titanium in this system.

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Date submitted: 30 Nov 2007

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