The Titanium-Boron Nitride interaction

GERARDO J. VAZQUEZ, FERNANDO MAGANA, EDUARDO RANGEL, GREGORIO RUIZ, Instituto de Física — 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.