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Seminaires du LPTM , Universite de Cergy Pontoise

Jeudi 27 Fevrier 2020, 14 :00
LPTM, 4.13 St Martin II
Domaines : cond-mat

Titre : *Structural and electronic properties of graphene/mos 2 heterostructures*

Orateur : **Venkateswarlu Somepalli (LPTM CY Cergy Paris Université, Cergy Pontoise.)**

Résumé : *We report the structural and electronic properties of the graphene/MoS 2 bilayer heterostructures, for theoretical study calculations we used Density functional theory [Abinit] with Van der Waals corrections. We analyze the interlayer spacing between the graphene and MoS 2 layers and also the charge transfer between the layers. In particular, we focus on the structural and electrical properties of bilayer heterostructures with different supercell geometries, with and without optimized bilayer heterostructures. These heterostructures are created with different supercell geometries like graphene (4x4)/MoS 2 (3x3) [4 :3], graphene (5x5)/MoS2(4x4)[5 :4] and graphene (9x9)/MoS2(7x7)[9 :7] having different magnitudes of lattice mismatch.*