CONTROL ID: 2042381
CONTACT (NAME ONLY): Angel Rubio
Abstract Details

PRESENTATION TYPE: Invited Speaker
CURRENT SYMPOSIUM: J. Emerging Non-Graphene 2D Atomic Layers and van der Waals Solids
KEYWORDS: Properties/Transport/electrical properties.
Abstract

TITLE: Novel electronic and structural properties of two-dimensional materials: silicene, germenene and stanene
AUTHORS (FIRST NAME, LAST NAME): Angel Rubio[1, 2]
INSTITUTIONS (ALL):
1. Materials Science, University of the Basque Country, San Sebastian, Spain.
2. European Theoretical Spectroscopy Facility (ETSF), Donostia, Spain.
ABSTRACT BODY:
Abstract Body: Based on first-principles calculation we predict two new thermodynamically stable singel and multi-layered-phases of silicon which exhibit strong directionality in the electronic and structural properties. As compared to silicon crystal, they have wider indirect band gaps but also increased absorption in the visible range making them more interesting for photovoltaic applications. Moreover, the intrinsic two-dimensional confinement and strong electron-phonon coupling make them a candidate material for thermoelectricity and superconductivity. These stable phases consist of intriguing stacking of dumbbell (DB) patterned silicene layers having trigonal structure with √3×√3 periodicity of silicene. We propose a new mechanism for explaining the spontaneous and consequential formation of √3×√3 structures from 3×3 structures on Ag substrate. We show that the √3×√3 reconstruction is mainly determined by the interaction between Si atoms and have weak influence from Ag substrate. The proposed mechanism opens the path to understanding of multilayer silicon and silicites.
We extended those studies to Ge and Sn. For the case of Ge, we showed that single and multi--layer germanium grow on a gold (111). Its growth bears strong similarity with the formation of silicene layers on silver (111) templates. One of the phases shows a clear, nearly flat, honeycomb structure. Thanks to thorough synchrotron radiation core-level spectroscopy measurements and advanced Density Functional Theory calculations we identify it to a √3x√3R(30°) germanene layer in coincidence with a √7x√7R(19.1°) Au(111) supercell.
For the case of Sn, we predict from the first-principles calculations that the stanene with dumbbell units (DB) is a fully stable two-dimensional (2D) topological insulator with inverted bands around the Γ point and its band-gap can be tuned by compressive strain. The quantum anomalous Hall effect, Chern half metallicity and topological superconductivity are possible to be observed in DB stanene
boron nitride sheet and reconstructed (2×2) InSb(111).

Acknowledgements: This work was supported by the European Commission within the FP7 CRONOS project (ID 280879), the European Research Council Advanced Grant DYNamo (ERC-2010-AdG-267374), Spanish Grant (FIS2010-21282-C02-01), Grupos Consolidados UPV/EHU del Gobierno Vasco (IT578-13)

Work done in collaboration, joint <b style="line-height:1.6em">Publications:/b>
Germanene: a novel two-dimensional Germanium allotrope akin to Graphene and Silicene, M.E. Dávila, L. Xian, S. Cahangirov, A. Rubio, G. Le Lay (2014)
Silicite: The new layered allotrope of silicon, S. Cahangirov, V. Ongun Özçelik, A. Rubio, S. Ciraci (2014)

The atomic structure of the √3×√3 phase of silicene on Ag(111), S. Cahangirov, V. O. Özçelik, L. Xian, Jose Avila, S. Cho, M.C. Asensio, S. Ciraci, A.l Rubio (2014)

Stable two dimensional dumbbell stanene: a quantum spin Hall insulator, P. Tang, P. Chen, W. Cao, H. Huang, S. Cahangirov, L. Xian, Y. Xu, SC. Zhang, W. Duan, A. Rubio (2014)

(no table selected)