

XXIII Latin American Symposium on Solid State Physics

Simposio Latinoamericano de Física del Estado Sólido XXIII



SLAFES XXIII
Bariloche

Bariloche, 10 - 13 April 2018

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PWQ-VI-6

Thermodynamic properties of Pt nano-clusters: an ab initio study

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Nanoparticles (NPs) exhibit novel physical and chemical properties that differ significantly from their counterpart bulk materials. Concerning thermodynamic properties, there are still fundamental questions not yet resolved. Anomalous behaviors in NP thermodynamic properties were reported, such as deviations from the Debye law of the specific heat and negative thermal expansion [1, 2]. The Debye temperature (θ_D) is a fundamental property, closely related to changes in the vibrational properties and specific heat. For capped Pt NPs θ_D was measured by extended X-ray absorption fine structure, leading to values higher than for the bulk [3]. For subnanometer Pt NPs (0.9 ± 0.2 nm and $N_{avg} \sim 16$ atoms) supported on Al_2O_3 experimental studies based X-ray absorption spectroscopy exhibit marked contractions of the Pt-Pt bond distances with respect to the bulk, and a negative thermal expansion of the interatomic distances [2]. The surface atom contraction and the interaction of the Pt atoms with capping molecules or support, were indicated as possible reasons to explain these anomalous behaviors. As a first step to investigate these problems, in this work we calculate ab initio the thermodynamic properties of isolated Pt NPs for sizes between 13-55 atoms. We expect to shed some light on the problem by considering only the intrinsic effects of the small dimension of NPs. From the determined NPs equilibrium geometries, we evaluate their vibrational density of states (VDOS), and the specific heat. The thermal evolution of the average interatomic distances is determined by ab initio molecular dynamics. We find that the relaxed interatomic distances are reduced with respect to the bulk ones. The VDOS present discrete states giving rise to deviations from the typical Debye model of the specific heat at low temperatures. Estimated θ_D are lower than for the solid.

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PWQ-VI-7

Tuning the topological states in metal-organic bilayers

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We have investigated the energetic stability and the electronic properties of metal-organic topological insulator bilayers (BLs), (MC4S4)3 BL, with M = Ni and Pt, using first-principles calculations and tight-binding model. Our findings show that (MC4S4)3 BL is an appealing platform to perform electronic band structure engineering, based on the topologically protected chiral edge states. The energetic stability of the BLs is ruled by van der Waals interactions, the AA stacking being the energetically most stable one. The electronic band structure is characterized by a combination of bonding and antibonding kagome band sets, revealing that (NiC4S4)3 BL presents a Z2 -metallic phase, whereas (PtC4S4)3 BL may present Z2 -metallic phase or quantum spin Hall phase. Those nontrivial topological states were confirmed by the formation of chiral edge states in (MC4S4)3 BL nanoribbons. We show that the localization of the edge states can be controlled with a normal external electric field, breaking the mirror symmetry. Hence, the sign of electric field selects in which layer each set of edge states are located. Such a control on the (layer) localization of the topological edge states brings us an additional and interesting degree of freedom to control the transport properties in layered metal-organic topological insulators.

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PWQ-VI-8

Magnetic-optical transitions induced by twisted light in quantum dots

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Twisted light (TL) is light having a helical wave front. Such light exhibits several interesting features: Due to the azimuthal phase dependence a phase singularity occurs at the beam axis, leading to the name optical vortex. Furthermore, in addition to spin angular momentum (SAM) associated with the handedness of circular polarization, such light fields carry