Seminario di Dipartimento
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DFT calculations to better understand solid materials on microscopic scale

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Abstract

In the last 25 years DFT calculations became an important tool for better understanding of different phenomena on microscopic level, which is not always evident from experimental study in the Physics, Chemistry and Material Science [1].
Especially in Material Science this kind of calculation can give us more open picture on diffusion, defect formation on the surfaces and in the bulk and some heterogeneous catalysis data. A key task of computational materials science is to unravel the often hidden composition-structure-property relationships on atomic level using computational techniques [2].
This conference is aimed to demonstrate and popularize the DFT calculations. Its goal is not only to present just the series of results but also show which rich spectra of results could be obtained working on the computer in the office and discuss the actual limits of this calculations.
In this talk will be presented the results on bulk:

- Study of vacancy formation and their diffusion in iron [3]
- Study of fundamental properties of Fe16C2 phase in the steal [4,5]

And the results on surface:

- Quasicrystalline approximant o-$Al_{13}Co_4$ as a candidate for selective hydrogenation of acetylene [6,7].

References:

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[3] D. Kandaskalov, C. Mijoule, D. Connétable, J. Nucl. Mat. **441**, 168 (2013)
[4] D. Kandaskalov, P. Maugis, Comp. Mat. Sc. **128**, 278 (2017)
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[6] D. Kandaskalov, J. Ledieu, V. Fournée, É. Gaudry J. Phys. Chem. C **118**, 23032 (2014)
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