THEOS
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The mysteries of iron-carbon at the nano-scale and the high-throughput highway to computational materials design

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Abstract: Through practical examples, in the first part of the presentation we will explore the interplay between phases competing for stability at the nanoscale, focusing on their effects on catalytic reactions. By leveraging the complex interplay between surface-tension and surface-energy contributions, we will address: 1) reduced solubility in iron nano-catalysts and thermodynamic limit of nanotubes growth [1], 2) size-induced viscosity - the kinetic counterpart of dynamic coexistence - with "super-1/R" effects on reaction speeds (dynamic renormalization of the time frame) [2], and 3) self-consistent variational approaches to the hierarchy of shape of nano-catalysts [3]. In the second part of the presentation, the high-throughput computational materials design will be introduced as one of the main enablers of the materials genomics initiative [4,5]. The key for discovering new materials is the availability of descriptors: physically-sound empirical quantities. A snapshot of this rapidly evolving field will be given and our most recent contributions will be discussed for thermoelectricity [6,7], topological insulation [8], and rare-earths strategic/critical materials replacement [9].

[1] Phys. Rev. Lett. **100**, 195502 (2008)
[2] ACS-Nano **4**, 6950 (2010)
[3] ACS-Nano **5**, 247 (2011)
[4] Nature Mater, **12**, 191 (2013).
[5] http://aflowlib.org .
[6] Phys. Rev. X **1**, 021012 (2011).
[7] Open-Heusler project.
[8] Nature Materials **11**, 614 (2012)
[9] *www.defense.gov/news/2013MURITeams.pdf "MURI Topological Decompositions and Spectral Sampling Algorithms for Elements Substitution in Critical Technologies".*