Case-Studies for Computer-aided Materials Design: alloyed Hausmanites and Gold Nanoparticles

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We employ hierarchical multi scale calculations, with Density-Functional Theory (DFT) coupled to continuum models and machine learning algorithms, in order to unravel the transport mechanism in manganese oxide alloys and provide methodology for reliable edge-energy calculation for metal nanoparticles.

We study Mn_3O_4 alloyed with Zn and Ni, both in the Hausmanite and the inverse spinel structures. Experimental investigation has shown that these alloys exhibit impressive non-Arrhenius dependence of conductivity on temperature, and can thus be used as temperature sensors. The experimental results can be explained through extensive DFT calculations coupled to a model of polaron hopping in an inhomogeneous energy landscape [1] .

We calculate edge energies of gold nanoparticles using a data-informed machine-learning (ML) multiple linear regression algorithm. The algorithm was provided with structural data for the nanoparticles along with the total energy as was calculated using either interatomic potentials or Density Functional Theory (DFT). The predicted edge energies are well converged with respect to the sample size. Moreover, we present for the first time vertex energies of gold nanostructures [2].

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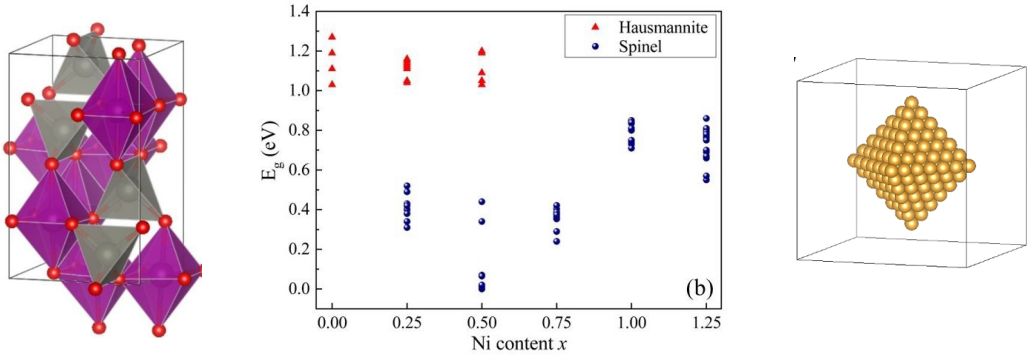

Figure 1: Left: The Hausmanite crystal structure. Center: Calculated band-gaps of the most stable structures for $Zn_{0.5}Ni_xMn_{2.5-x}O_4$. Right: An octahedral Au nanoparticle.

References

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