DFT modeling and transport properties of PdGa and PdIn compounds

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Intermetallic compounds are innovative catalyst materials. Their potential lies in spatial separation of active sites which enables high activity and selectivity.[1] Furthermore, it is possible to change their electronic properties by tuning their chemical composition. Palladium based intermetallic compounds, particularly PdGa and PdIn have shown very good catalytical properties in partial hydrogenation of acetylene to ethylene and methanol steam reforming processes respectively. Although catalysis occurs on the surface, it is important to know properties of the bulk as well. In order to get a deeper insight into those systems we calculated their electronic and vibrational spectra within density functional theory (DFT) using Quantum ESPRESSO [2] and WIEN2k code [3]. Detailed analysis of their experimental transport properties with correlation to the electronic structure will be presented.[4] We extracted scattering rates of different bands by the use of experimental transport properties. From vibrational spectra and electrical resistivity we successfully estimated Debye temperature and correlated it to the specific heat results.

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