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Uni- and bi-metallic small Pt and Ni clusters for fuel conversion applications: A DFT study

An ab initio density functional theory study was performed to investigate the adsorption of C and OH on small uni-metallic (Pt3 and Ni3) and bi-metallic (Pt2Re and Ni2Fe) clusters that could be potentially used for energy conversion applications. We observed that the HOMO-LUMO gaps show good stability and reactivity of the clusters. Furthermore, the introducing foreign atoms (Re and Fe) provides useful insights in designing and fine-tuning of these catalysts for energy conversion applications such as CO/CO2 methanation and hydrogenation reactions. Moreover, we observed that Pt3 and Pt2Re clusters bind with C and OH moderately, which could be utilized further for energy conversion.

Reference:
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