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Effect of adsorbates on the isomer stability of Ir_4 clusters

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The relative stability of Ir_4 isomers, both in the gas phase and on MgO(100) substrate, is studied using density functional theory. The square Ir_4 is the most stable in both cases. The metastable tetrahedral isomer, which experimental data suggest as the most stable form of Ir_4 on MgO(100), is highly distorted by the strong Ir–O interactions. The relative stability of Ir_4 isomers is strongly altered by adsorption of a single C atom since the binding energy of the C adatom to tetrahedral and butterfly Ir_4 is much larger (~ 1.7 eV) than that to the square one, both in the gas-phase and on MgO(100). After carbon adsorption, the most stable structure of Ir_4 is the butterfly geometry for free clusters and the "tetrahedral" one for Ir_4/MgO(100). The C adatom binds in a bridge configuration in all cases and reduces the distortions produced by the MgO substrate. Energetics and equilibrium atomic geometries will also be discussed for the adsorption (*i*) one H or O atom and (*ii*) one CO molecule.

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