Modified New Carbon K4 and Metal-Organic Framework Structures: A Theoretical DFT Study

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In the present talk we would like to bolster advantages of the cluster approach (being relatively very simple but complementary to other periodic slab model calculations) in proper modeling of extended systems [1-3]. Especially, the structure and chemical activity of the selected transition metal and metal oxide catalysts would be thoroughly discussed [3-5]. In line with combining of metal oxide connectors with organic linkers into extended metal-organic framework (MOF) networks, some solutions is given to stabilize and characterize modified new carbon K4 [6] and related new IRMOF structures. Based on these DFT cluster calculations results, some discrepancies with the results of other theoretical investigations and studies in literature have been critically pointed out.

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