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The adsorption of CH_3 and C_6H_6 on corundum-type sesquioxides: The role of van der Waals interactions SAMIRA DABAGHMANESH, Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Antwerp, Belgium., BART PARTOENS, Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium., ERIK NEYTS, Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Antwerp, Belgium. — Van der Waals (vdW) interactions play an important role in the adsorption of atoms and molecules on the surface of solids. This role becomes more significant whenever the interaction between the adsorbate and surface is physisorption. Thanks to recent developments in density functional theory (DFT), we are now able to employ different vdW methods that helps us to account for the long-range vdW forces. However, the choice of the most efficient vdW functional for different materials is still an open question. In our study, we examine different vdW approaches to compute bulk and molecular adsorption properties of M_2O_3 oxides (M: Cr, Fe, and Al) as well-known examples of the corundum family. For the bulk properties, we compare our results for the heat of formation, cohesive energy, lattice parameters and bond distances as obtained using the different vdW functionals and available experimental data. Next we compute the adsorption energies of the benzene molecule (as an example of physisorption) and CH_3 (as an example of chemisorption) on top of the (0001) M-terminated and MO-terminated surfaces. Calculating the vdW contributions into the adsorption energies, we find that the vdW functionals play important role not just in the weak adsorptions but even in strong adsorption.

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