Tailoring Metal-organic frameworks for adsorption applications

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Resume : Metal-organic frameworks (MOFs), also referred to as hybrid organic-inorganic materials, have emerged as a class of highly tunable crystalline materials showing ultrahigh porosity and internal surface areas. These materials consist of two secondary building units (SBUs): (1)metal(-oxide) nodes are connected through (2)organic ligand molecules. The variability of the SBUs allows an almost limitless set of possible combinations, each having its own specific properties. In addition, functional groups can be added to the linkers giving rise to modified host-guest interactions. The resulting MOFs are of great interest for many important industrial applications such as clean energy, hydrogen storage and carbon-dioxide capture. Also catalysis, gas-separation and sensor applications are fields of interest. In this work, we present an ab-initio study of functionalized MIL-47(V) MOFs. We show how different linkers influence the stability of the MOF and its adsorption of CO2. Using the Hirshfeld-I scheme charge transfer between the SBUs and the functional groups is discussed. Finally, a protocol is given for calculating high quality mechanical properties (e.g. bulk moduli) and vibrational spectra, providing thermal contributions to the energy. [1]Biswas S., Vanpoucke D.E.P., et al., J. Phys. Chem. C 117,22784-22796(2013) [2]Vanpoucke D.E.P., Bultinck P.,and Van Driessche I.,J. Comput. Chem. 34,405-417(2013) [3] Ghysels A.,Vanpoucke D.E.P.,Lejaeghere K.,et al., in preparation