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**Spectroscopic studies of van der Waals bonding and interactions in microporous materials<sup>1</sup>**

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Van der Waals interactions govern the interaction of gas phase molecules in microporous materials. New theoretical approaches, such as DF-vdW methods, have brought great insight into the results of vdW forces on the adsorption and diffusion properties of molecular guests. In this talk, we highlight the role of vibrational spectroscopies (infrared and Raman) in providing information that can directly test such theoretical approaches. Typically, vdW interactions lead to measurable shifts in molecular internal modes, which can be calculated. We also show that vdW interactions often lead to minor structural alteration or reconfiguration of the microporous hosts, which can clearly be observed by IR or Raman spectroscopy. Examples will be taken from molecular hydrogen storage and gas phase separation in Metal Organic Framework materials, which represent a versatile class of porous materials. For example, the origin of interesting “gate opening” phenomena in flexible MOFs, leading to highly selective adsorption, will be described.

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