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**Rotational and vibrational excitations of van der Waals bonded hydrogen in nanoporous materials:
calibrating first-principle calculations with experiments¹**
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The adsorption of H₂ within a metal-organic framework is studied via van der Waals density-functional calculations and maximally-localized-Wannier- function analysis. The calculated low-lying vibrational and rotational energy states as well as the adsorption sites are consistent with experiments. The induced dipole due to H₂ bond stretching and its quantum mechanic matrix element is found to be accurately given by a first-principles driven approximation. The resulting calculations of IR intensity explain the experimentally mysteriously missing primary line for para hydrogen. The strengths and positions of lines in the complex spectra of rotational-vibrational transitions are in reasonable agreement with experiment, and a selection rule is obtained.

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