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**Three-body interactions in liquid and solid hydrogen:
Evidence from vibrational spectroscopy** ROBERT HINDE, Univ.
of Tennessee — In the cryogenic low-density liquid and solid phases of H₂
and D₂, the H₂ and D₂ molecules retain good rotational and vibrational
quantum numbers that characterize their internal degrees of freedom.
High-resolution infrared and Raman spectroscopic experiments provide
extremely sensitive probes of these degrees of freedom. We present here
fully-first-principles calculations of the infrared and Raman spectra of
liquid and solid H₂ and D₂, calculations that employ a high-quality six-
dimensional coupled-cluster H₂-H₂ potential energy surface and quan-
tum Monte Carlo treatments of the single-molecule translational degrees
of freedom. The computed spectra agree very well with experimental re-
sults once we include three-body interactions among the molecules, in-
teractions which we also compute using coupled-cluster quantum chem-
ical methods. We predict the vibrational spectra of liquid and solid H₂
at several temperatures and densities to provide a framework for inter-
preting recent experiments designed to search for superfluid behavior
in small H₂ droplets. We also present preliminary calculations of the
spectra of mixed H₂/D₂ solids that show how positional disorder affects
the spectral line shapes in these systems.

Prefer Oral Session
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