SUPERFLUID EFFECTS IN PARA-H_2 CLUSTERS PROBED BY CO_2 ROTATION-VIBRATION TRANSITIONS

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The prospect of directly observing superfluidity in para-H_2 is a tantalizing but elusive goal. Like ^{4}He, para-H_2 is a light zero-spin boson. However, H_2-H_2 intermolecular interactions, though weak, are stronger than He-He interactions, and hydrogen is a solid below about 14 K. This makes detection of superfluidity in bulk hydrogen problematical, to say the least. But there are still possibilities for para-H_2 in the form of clusters or in nano-confined environments, and superfluid transition temperatures as high as $\sim$6 K have been predicted.[a] Spectroscopic observations of (para-$H_2)_N$-CO_2 clusters[b] were at first very difficult to interpret for $N > 5$. However, with the help of path integral Monte Carlo simulations and an accurate new H_2-CO_2 intermolecular potential surface[c] which explicitly incorporates dependence on the CO_2 ν_3 asymmetric stretch, it is now possible to achieve a remarkably consistent picture of (para-$H_2)_N$-CO_2 clusters in the size range N = 1 $\sim$ 20. By combining the experimental spectroscopic measurements and theoretical simulations, we determine the size evolution of the superfluid response of the CO_2-doped para-H_2 clusters, which peaks for the "magic" number N = 12.

[a] V.L. Ginzburg and A.A. Sobyanin, *JETP Lett.* **15**, 343 (1972).
[b] A.R.W. McKellar, Paper WH04, 63rd OSU International Symposium on Molecular Spectroscopy, June 16-20, 2008.
[c] H. Li, P.-N. Roy, and R.J. Le Roy, *J. Chem. Phys.*, submitted.