Quantum ionic effects in high-temperature superconducting hydrides at high pressure

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The discovery of superconductivity in H_3S at approximately 200 K and in LaH_{10} at 250 K [1,2,3], in both cases at a pressure of around 150 GPa, clearly shows that hydrides provide a realistic route towards the long-standing dream of room temperature superconductivity. At least at high pressures.

First-principles crystal structural prediction methods, which seek for phases in the minimum of the Born-Oppenheimer energy surface, have turned extremely useful to guide experimental work in the right track. A clear example of it is the LaH_{10} case, which seems to superconduct at such high temperatures in a beautiful sodalite structure that was predicted by first-principles calculations before [5,6]. However, the problem of these methods is that they do not consider the quantum ionic zero-point energy in the calculations, which is expected to be very large for these compounds with high hydrogen content.

In this talk I will show that indeed the Born Oppenheimer energy surface is strongly affected by the quantum effects associated to the ionic vibrations, often completely changing the minima obtained at the static or classical level. Ionic quantum effects therefore do not only imply a huge anharmonic correction in the phonon spectrum, which can stronly impact the superconducting critical temperatures [6], but also in the crystal structures and the chemichal bonding itself. I will illustrate that indeed these quantum effects are crucial in both H_3S and LaH_{10} high-temperature superconductors.

Our results have large implications for the fate of crystal structure predictions that stick to mapping the Born Oppenheimer energy surface at a classical level.

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