Record superconductivity in the sulfur hydride system

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The recent discovery by Drozdov et al. [1] of superconductivity at 200 K in hydrogen sulfide compressed to about 150 GPa breaks the record of the cuprates and overturns the conventional wisdom that such a high critical temperatures cannot be obtained via phonon-mediated pairing. This extraordinary measurement is the first experimental proof that high-temperature superconductivity can be attained at high pressure in hydrogen-rich compounds, as proposed by Ashcroft [2,3]. Exciting new prospects are now open to find room temperature superconductivity in other hydrogen-rich materials. This will stimulate a new experimental and theoretical effort to discover new hydrides that might overtake the superconducting record recently set by hydrogen sulfide.

In this talk I will underline that in order to characterize form theoretical first-principles techniques the structural, chemical, electronic, and vibrational properties of these hydrides, it is crucial to properly include the quantum nature of the protons in the calculations. According to our *ab initio* calculations based on density-functional theory [4,5,6], in the record hydrogen sulfide superconductor the quantum nature of the proton and the consequent huge anharmonicity strongly alter the nature of the hydrogen bond, make the solid adopt a crystal structure that is not the minimum of the static Born-Oppenheimer energy surface in a given pressure range, and dramatically modify the vibrational spectra. Interestingly, such strong quantum effects are necessary ingredients to understand the superconducting properties in this system.

Our results suggest, therefore, that the quantum nature of the proton needs to be included in theoretical calculations seeking for new hydrides with potential high-temperature superconductivity, not only for determining their vibrational spectra and superconducting properties, but even for determining the crystal structure and the hydrogen bonding.

Bibliography:

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