High-temperature superconductors, the interesting case of PdCuHx ternary hydride

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The discovery of electron-phonon mediated high-temperature superconductivity in hydrogen-rich materials (*e.g.* H_3S[1] and LaH [2]) represents a milestone in condensed matter physics: for the first time it was possible to have a glimpse to room temperature superconductivity, marking the beginning of a new era.
In fact, within a few years (in 2022) room-temperature superconductivity was finally achieved in C-S-H ternary compound at P≈270GPa (T_C=287K)[3]. This discovery is extremely important demonstrating that ternary superconducting hydrides can also be stabilized, broadening the spectrum of possibilities to search for new promising superconductors, which may also be stable at lower pressure.

Interestingly, the hydride topic is an old one in condensed matter physics. In fact, the first superconducting hydrides were discovered at ambient pressure in 1970s in Th_4H [4] and, in particular, in palladium hydride (PdH)[5]: a binary compound with T_C=8-9K. Although with a small critical temperature, this last system was reported[6] (in 1974) to significantly increase the value of T_C (up to two times its original value) if alloyed with noble metals like copper, silver or gold. Almost 50 years has passed, but the mechanism responsible for this unusual behavior was still unknown.
In this context, I present an *ab initio* study of the ternary hydride $PdCuH_x$ [7], a parent compound of the superconducting PdH, at different hydrogen content (x=1,2). I present its structural, electronic, dynamical, and superconducting properties, demonstrating that, at low hydrogen content, the system is not a superconductor above 1 K; however, the highly hydrogenated structure is a strongly coupled superconductor. I give a solid rationale for the unusual increase of the superconducting critical temperature in hydrogenated palladium when alloyed with noble metals (Cu, Ag, and Au), as observed in Stritzker's experiments in 1974[6] but never investigated with modern experimental and theoretical techniques.

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