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Towards an ab initio theory of high-temperature superconductors: a study of multilayer cuprates

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A new quantum framework reveals how chemistry and crystal structure govern high-temperature superconductivity, explaining behaviors seen in multilayer cuprates and guiding the search for room-temperature superconductors.

While low-temperature superconductivity is well understood, the mechanisms behind superconductivity at higher temperature remain elusive. In this work, we propose a quantum mechanical framework aimed at identifying the key chemical elements and crystal structures needed to design new materials that superconduct at or near room temperature. The framework is based on Density Functional Theory plus Cluster Dynamical Mean-Field Theory.

To demonstrate our approach, we apply it to two families of copper-oxide superconductors known as multilayer cuprates. These materials hold the record for the highest superconducting temperatures at ambient pressure. Using our model, we explain why superconducting properties depend on the number of superconducting layers, why mercury-based cuprates outperform calcium-based ones, and how magnetism, electronic structure, and charge distribution influence superconductivity. Our predictions align closely with experimental observations, showing the strength of this method in capturing complex material behaviors.

This work lays the foundation for a comprehensive, first-principles understanding of high-temperature superconductors. Looking ahead, we aim to extend our method to large-scale computational searches and apply it to other classes of materials, such as nickelates and pnictides. By doing so, we move closer to the long-standing goal of designing a superconductor that operates at room temperature.

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