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Computational search of novel superconductors

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The recently discovered 200 K high temperature superconductivity in the hydrogen sulfur material under high pressure was first successfully predicted by first-principles computation in a quantitative fashion, demonstrating the power of computation in the search of new superconductors. With the rapid advancement of theory, algorithm, and computer power, computation will play an increasingly important role. In this talk, I will first summarize the key features of different families of high temperature superconductors, including the iron pnictide and chalcogenide superconductors, the transition metal chloronitrides, and Bi-based superconductors. Then I will show how to use the key features as guidance to design novel candidate materials of high temperature superconductivity by utilizing a combination of different computational methods and tools, including evolutionary structural search method, density functional theory and dynamical mean field theory. A few candidate materials will be given towards the end of the talk for interested experimentalists and theorists to test and explore