

From electron delocalization to predicting superconductivity

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A room temperature superconductor is probably the most desired system in solid state physics. So far, the greatest advances, cuprates, pnictides and number of others were obtained in a serendipitous way. As there is no clear theory for these superconductors, it is difficult to predict where progress will be made. In contrast the Bardeen-Cooper-Schrieffer (BCS) theory gives a clear guide for achieving high T_c , and hydrogen seems to be a main clue. Within this approach, the recently reported superconductivity at 190 K in compressed H₂S [1] has been arguably the biggest discovery in the field since the superconducting cuprates nearly 30 years ago.

However, a microscopic understanding of why this particular material features such a strong coupling is still missing. We have recently shown that the underlying chemical structure and bonding need to be characterized for a good comprehension of the chemical composition-superconductivity relation.

We have resorted to superconducting DFT within Tight Binding models showing that the normal state DFT can be used to characterize the bonding in superconductors. Based on these results, we have defined two global quantities derived from the Electron Localization Function [2] which characterize i) the molecularity and ii) the metallicity of hydrogen compounds [4].

We have constructed a database of binary and ternary hydrogen-based compounds with available critical temperatures and shown that these two indexes allow to characterize i) the type of crystal and ii) its superconducting nature (critical temperature), respectively. Thanks to machine learning algorithms (decision trees), a very good correlation has been obtained for predicting superconducting critical temperature in all these compounds. This goes beyond our initial proposition [3] which was only applicable to binary compounds.

These developments are now available at a public code, Tcetime [5]; which allows to predict in a simple and fast manner the critical temperature from a DFT calculation. A server to make this calculation online will also soon be available. We hope that these developments will open the possibility for a real high-throughput screening of new potential low pressure high critical temperature superconductors and, at the same time, sets clear paths for chemically engineering better superconductors.

References

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