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Classification of metal polyhydride critical temperature using support vector machine

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The recent experimental and theoretical search for near-room temperature superconductors have shed light of interest on metal hydride as the critical temperature can vary from a few kelvins to over 200 kelvins. One problem occurring in the theoretical research of the material is that the traditional way of studying thermal superconductivity material is through calculation of electron-phonon spectral function which cost enormous amount of time and computational resource. Here we propose machine learning method (Support vector machine) to classify the critical temperature of the material without calculating electron-phonon spectral function. The features used in the model are based on electronic properties occur from hydrogen atom in the molecule and consideration effect of electron localization function which have strong correlation to the temperature, this set of features can be obtained faster and with less computational resources than directly find the critical temperature. Decision boundary from the model can categorize most material in the dataset and thus speed up the quest for future high-temperature hydrogen-based superconductors.

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