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Relating Debye and Superconducting Transition Temperatures by Machine Learning in Conventional Superconductors[1] ADAM SMITH, SUMNER HARRIS, RENATO CAMATA, CHENG-CHIEN CHEN, University of Alabama at Birmingham — Recently a relationship between the Debye temperature Θ_D and the superconducting transition temperature T_c of conventional superconductors has been proposed [in npj Quantum Materials **3**, 59 (2018)]. The relationship indicates that for phonon-mediated BCS superconductors the maximum T_c is at most $\sim 0.1 \times \Theta_D$. In order to verify this bound and develop tools for predicting the Debye temperature, we trained Machine Learning models on over 10000 compounds with just chemical formula and crystal system information as features. By examining 5000 known superconducting compounds in the NIMS SuperCon database, our predictions show that the conventional superconductors in the database indeed follow the previously proposed bound of T_c vs. Θ_D. We also discuss our manual selection criteria and Machine Learning clustering techniques to separate conventional superconductors from others in the NIMS SuperCon database.

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