**First-principles calculations and machine learning for designing advanced materials**

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Cuprates have been at the center of long debate regarding their superconducting mechanism; therefore, predicting the critical temperatures of cuprates remains elusive. On the other hand, the data-driven machine learning (ML) technique has been developed to predict the properties of materials without demanding a pre-known exact mechanism. Herein, using machine learning and first- principles calculations, we predict the maximum superconducting transition temperature (Tc,max) of hole-doped cuprates and suggest the functional form for Tc,max with the root-mean-square-error of 3.705 K and R2 of 0.969. We have found that the Bader charge of apical oxygen, the bond strength between apical atoms, and the number of superconducting layers are essential to estimate Tc,max. Furthermore, we predict the Tc,max of hypothetical cuprates generated by replacing apical cations with other elements. Among the hypothetical structures, the cuprates with Ga show the highest predicted Tc,max values, which are 71, 117, and 131 K for one, two, and three CuO2 layers, respectively. These findings suggest that machine learning could guide the design of new high-Tc superconductors in the future.