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Inverse Design of Materials by Multi-Objective Differential Evolution(IM^2ODE) YUE-YU ZHANG, Z.L. LI, H.J. XIANG, X.G. GONG, Fudan Univ — Inverse design is a new approach in the realm of material science for finding the structure with desired property. We developed a novel algorithm for inverse design named as IM^2ODE (Inverse Design of Materials by Multi-Objective Differential Evolution). The target properties of concern include optical and electrical properties of semiconductors, solar absorbers and hardness of materials. IM^2ODE can easily predict the atomic configurations with desired properties for crystal structures, interfaces and clusters. This novel method has been applied successfully in predicting new titanium dioxide (TiO_2) polymorph with optimal band gap for solar cell application.

Yue-Yu Zhang
Fudan Univ

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