How data mining can reduce computational complexity in the design of new materials

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Computational complexity in DFT calculations is crucial in the reliability of the calculated properties of materials. Computational cost of such methods is dominated by expensive first-principles determination of structural energies and atomic forces, including structural relaxations. Data mining is an opportunity to eliminate recalculation of known data, and, consequently, to reduce the total cost of calculations and can be extended for the prediction of any materials on the basis of those of the periodic table. We propose data mining as a universal tool for the design of new material. We show, that the DFT Database is a powerful tool for information integration and data mining, which can greatly reduce computational complexity in materials world.

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