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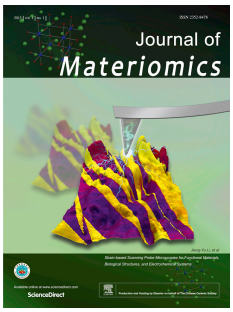

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Graphical Abstract

Data Mining-aided Materials Discovery and Optimization

Wencong Lu[1*], Ruijuan Xiao[2], Jiong Yang[1], Hong Li[2*], Wenqing Zhang[1*]

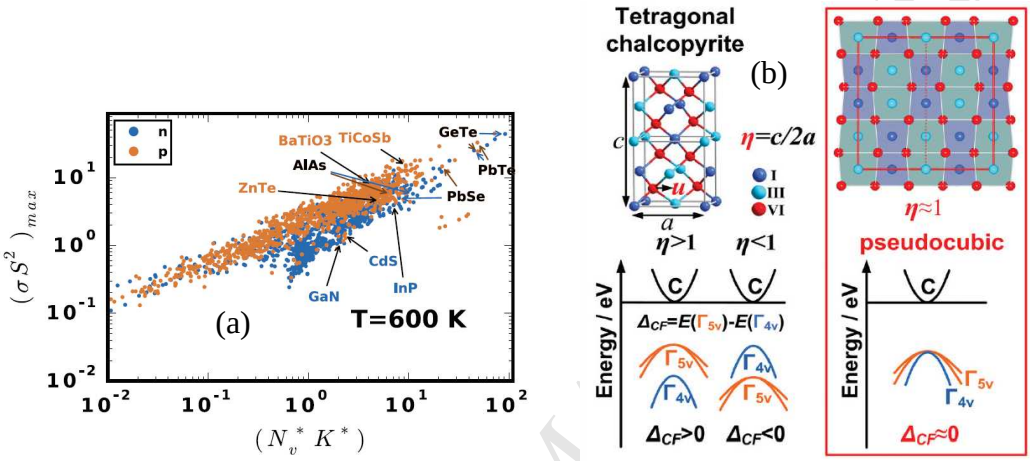

Fig. 10(a) The correlation between Nv^*K^* and the calculated power factors;[50] (b) the pseudocubic structure and converged band structures in tetragonal chalcopyrite compounds.[51]

Highlights—review paper

- Both qualitative and quantitative methods adopted widely in materials data mining (MDM) have been systematically reviewed to meet different tasks of materials discovery and optimization.
- The novel qualitative method by using optimal projection recognition technique is reviewed in detail for controllable synthesis of dendritic Co_3O_4 superstructures based on pattern recognition classification diagram.
- The detailed MDM process has been demonstrated in case study on materials design of layered double hydroxide with desired basal spacing based on the quantitative modelling method called relevance vector machine.