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Role of Features in the Adaptive Design of Materials PRASANNA V. BALACHANDRAN, TURAB LOOKMAN, Los Alamos National Laboratory —
In materials informatics, features or descriptors that capture trends in the structure, chemistry and/or bonding are crucial. Here, we explore their role in the accelerated search for new materials with a targeted response. To accomplish the objective, we construct two datasets that uses two sets of features (ionic radii and electronegativity) and independently track their progress to determine which of the two would rapidly find the optimal composition with the largest band gap (E_g). We model the feature–E_g relationship using support vector regression (SVR), which we subsequently utilize for predicting the E_g for the unexplored compositions with uncertainties. Our results show that the ionic radii feature set, despite its relatively poor model fit and large uncertainties, performed better and found the optimal material in fewer iterations compared to the electronegativity feature set, which intriguingly had superior model fit. Visualization of the SVR response surface showed that the the ionic radii feature set led to a far greater exploration of the chemical space, which we attribute as an important diagnostic for accelerated search.

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