RUHR-UNIVERSITÄT BOCHUM
FAKULTÄT FÜR PHYSIK UND ASTRONOMIE

PHYSIKALISCHES KOLLOQUIUM

Sommersemester 2022

Montag, 13.06.2022, 12 Uhr c.t. im HNB und
hybrid als Zoom meeting (Meeting-ID: 632 5520 9938, Passwort: 526977)

Machine-learning material properties with domain knowledge of the interatomic bond

Antrittsvorlesung

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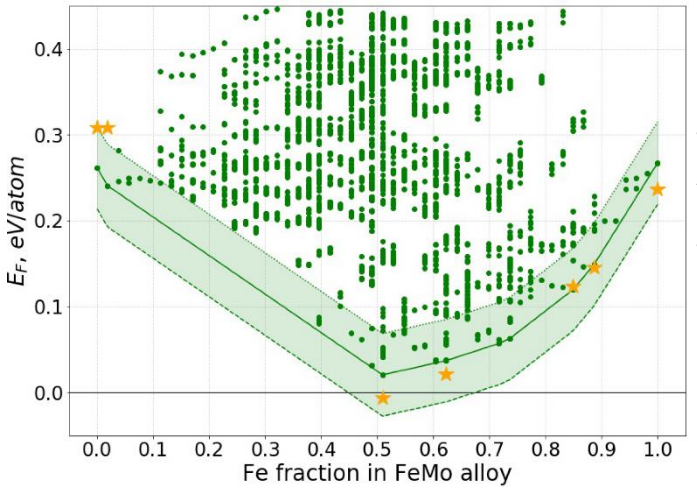

The computational design of materials relies on the ability to predict the stable atomic structure for a given chemical composition. At the atomic scale, electronic-structure calculations like density-functional theory (DFT) provide robust predictions but are often limited in the exploration of chemical diversity and geometric complexity due to the numerical effort. An increasingly important approach to overcome this limitation is modern data science with numerical representations of structure-property relationships. These are established by associating digital representations of atomic structures with their formation energies from DFT calculations and by a numerical representation of the relations in this data set by a machine-learning (ML) model.

The predictive power of the ML model strongly depends on the descriptors that represent the atomic structure. In this talk I will present recent developed descriptors that incorporate domain knowledge of the interatomic bond from a hierarchy of electronic-structure methods. The first level of domain knowledge uses simple model Hamiltonians to obtain the local density of states. The second level includes bond chemistry in terms of bond-specific model Hamiltonians from downfolded DFT eigenspectra. The third level picks up the influence of band filling via approximate bond energies. The application of these descriptors will be demonstrated for binary and ternary transition-metal alloys.

Einführung: Prof. Dr. Heiko Krabbe

Die Fakultät lädt alle Interessierten herzlich ein.