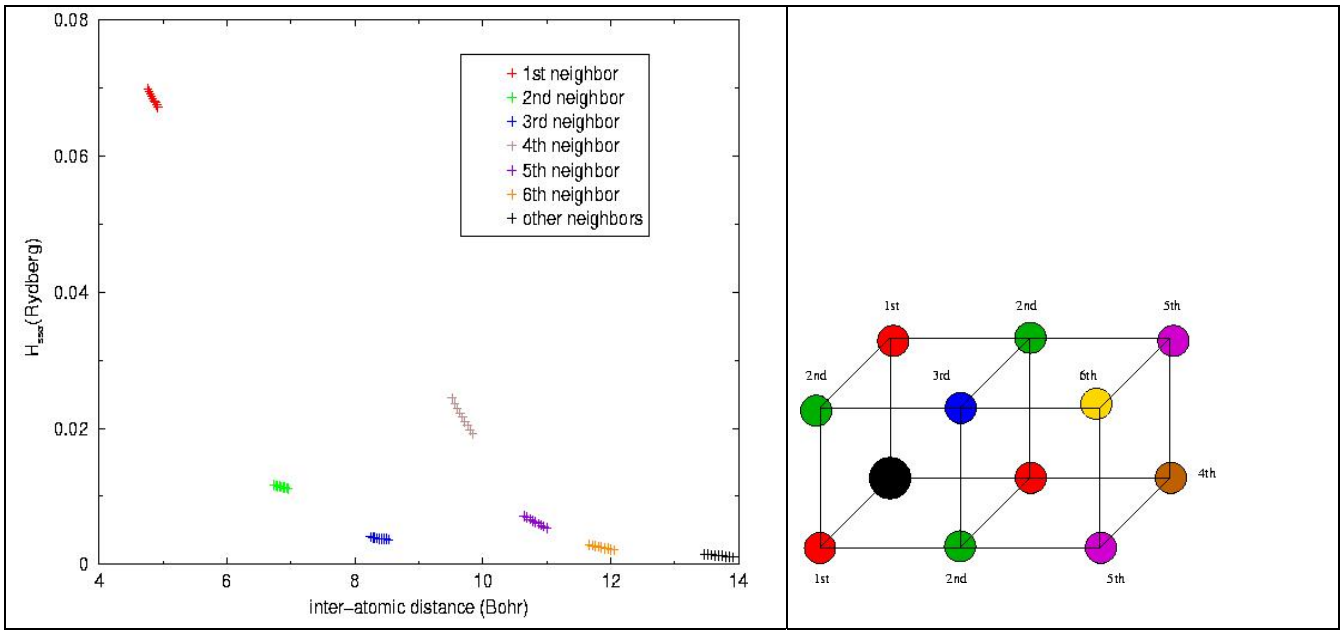

The ss- . tight-binding parameter for cubic Mo as a function of inter-atomic distance. The non-smoothness of the curve is due to the three-center (crystal fields) effects that are not accounted for in the original McMahan and Klepeis' approach, indicating that modification is necessary.

Integrated Research for Predicting Higher Dimensional Phase Diagrams With Emphasis on Ternary Diagrams of Molybdenum, Silicon, and Boron

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The objective of this project is to develop and evaluate behavior of molybdenum silicide alloys for land-based power plant turbines able to withstand temperature exceeding 1000ºC. In addition to relevant experimental work, the major task is computational modeling studies of ternary system of Molybdenum, Silicon and Boron over a wide range of temperature.

We are working on a new scheme of obtaining tight-binding (TB) parameters directly from ab-initio quantum mechanic calculations. The essence of this approach is to avoid the difficulties encountered by conventional numerical fitting methods, especially in the modeling of intermetallic compounds where the number of parameters is large. Starting from the Hamiltonian and overlap matrix elements that are prepared by full-potential linear muffin-tin orbital method, we obtain the intersite TB parameters using a modified McMahan and Klepeis's approach. The modification includes calibration of energy reference and employment of three-center interaction terms. We are currently developing an iterative solution to obtain the on-site TB parameters and the repulsive energies. Compared to our previous treatment, the current method eliminates numerical fitting all together, and therefore will increase the mathematical definiteness and physical soundness of the resulting parameters.

Read more about this work