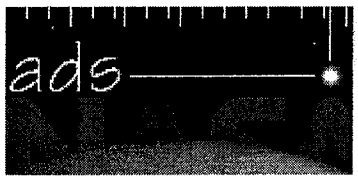

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Heats of Segregation of BCC Metals Using Ab Initio and Quantum Approximate Methods

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Many multicomponent alloys exhibit surface segregation, in which the composition at or near a surface may be substantially different from that of the bulk. A number of phenomenological explanations for this tendency have been suggested, involving, among other things, differences among the components' surface energies, molar volumes, and heats of solution. From a theoretical standpoint, the complexity of the problem has precluded a simple, unified explanation, thus preventing the development of computational tools that would enable the identification of the driving mechanisms for segregation. In that context, we investigate the problem of surface segregation in a variety of bcc metal alloys by computing dilute-limit heats of segregation using both the quantum-approximate energy method of Bozzolo, Ferrante and Smith (BFS), and all-electron density functional theory. In addition, the composition dependence of the heats of segregation is investigated using a BFS-based Monte Carlo procedure, and, for selected cases of interest, density functional calculations. Results are discussed in the context of a simple picture that describes segregation behavior as the result of a competition between size mismatch and alloying effects