

Abstract Submitted
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Modeling the effect of adsorbates on the surface segregation of binary alloy surfaces OLE M. LØVVIK, University of Oslo, SUSANNE M. OPALKA, United Technologies Research Center — The effect of adsorbed species on surface segregation in binary alloys has been investigated using band-structure density-functional theory. Particular emphasis is given to hydrogen adsorption on the Pd-Ag and Pd-Cu systems, which are of relevance for hydrogen selective dense metal membranes. It is demonstrated how adsorption can significantly alter the atomic-scale surface segregation in such binary alloy surfaces.

Ole M. Løvvik
University of Oslo

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