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Structural and Electronic Properties of Magnesium Hydride Surfaces. MICHEL A. POSTERNAK, ALFONSO BALDERESCHI, EPF–Lausanne, Switzerland — The Mg–MgH_2 system is of considerable interest in hydrogen technology, though the hydride forms very slowly. The microscopic mechanisms of hydriding/dehydriding Mg are not yet fully understood. In particular, transmission electron microscopy experiments[1] have shown differences in the relative orientation between the MgH_2 lattice and the (hexagonal) Mg substrate during the formation process $[\,(100)_{\text{hydride}} \parallel (0001)_{\text{Mg}}\,]$, and the decomposition one $[\,(110)_{\text{hydride}} \parallel (0001)_{\text{Mg}}\,]$. In order to contribute to the understanding of the above orientation differences, and in general of the reactions occurring at the MgH_2 surface, we have performed a comparative study of the unrelaxed and relaxed (100) and (110) surfaces. The electronic structure has been calculated using the LAPW method, and the chemical bonding has been obtained from the corresponding Wannier functions. Bonding at the surface differs from that of the bulk, and strongly depends on surface orientation and relaxation.

[1] B. Bokhonov *et al.*, Mat. Lett. **5**, 218 (1987); A. Altmann and T. Schober, Scripta Met. **25**, 723 (1991).

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