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Surface electronic structure of H/Li(110) – an application of the semi-infinite method.[1] YONAS ABRAHAM, N.A.W. HOLZWARTH, Wake Forest University — We report the application of our new semi-infinite method to study the Li (110) surface. This method calculates continuum and bound electronic states in the vicinity of a surface of a semi-infinite crystal. It is designed for solving the Kohn-Sham equations in a pseudopotential formulation, including both local and separable non-local contributions. It is based on the Numerov integration algorithm and uses singular value decomposition to control the exponentially growing contributions. For Li (110), we see that H changes the interference patterns of the continuum states. In addition, we are able to locate the energies of H-induced surface states relative to the bulk band edges. Comparison with supercell calculations of the same system, reveal interesting differences.

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