# Filling slab approach for the direct method: phonons for MgO(001) and Li/MgO(001) surfaces

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*Ab initio* calculations of surface phonons can be performed using the direct method[1]. This approach requires to know the Hellmann-Feynman forces computed in a supercell with a crystalline slab. Here, to increase the number of atoms in the simulated supercell a filling slab[2] approach is adopted. We show how to supplement in this case the Hellmann-Feynman force file calculated for a thin slab, by a similar force file from a bulk crystal, and use it in the direct method to find the phonon frequencies for a reasonable thick crystalline slab.

The approach is illustrated by *ab initio* slab calculations of phonons for MgO(001) and Li/MgO(001). Phonon dispersion relations[3] of the surface layer show the Raleigh modes and local Li vibrations. Phonon density of states of surface and middle layers show drastic differences for differently polarized vibrations. We acknowledge support of the EC under FP6 contract No. NMP4-CT-2003-001516 (DYNASYNC).

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[3] K. Parlinski, Phonon Software, Cracow (2005).