SELF-CONSISTENT CALCULATIONS OF THE SURFACE ELECTRONIC EXCITATIONS IN K(110) ADSORBED LAYER ON Be(0001) SUBSTRATE

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We investigate the collective surface excitations associated with an overlayer of K(110) atoms adsorbed on a Be(0001) substrate in the self-consistent jellium framework and with ab-initio pseudo-potentials calculations[1] in order to compare the results obtained from both approximations. We calculate the surface response function with energies and wave functions derived from the Kohn-Sham density-functional theory and from the non-conserving pseudo-potentials ab-initio calculations respectively. The dispersion relation for the plasmon modes[2], the real and imaginary part of the surface response function were obtained. A relation of the collective modes in Be surface and K/Be ad-layer surface is analyzed in terms of the contribution from each system.

References:

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