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Interface Electronic Structure and Possible Superconductivity in CuCl/Si(111)[1] S.H. RHIM, R. SANIZ, A.J. FREEMAN, Northwestern U., J. YU, Seoul National U. — To investigate a possible interfacial superconductivity [2] in CuCl/Si(111), we carried out electronic structure calculations using the highly precise FLAPW [3] method. As a result of charge transfer between CuCl and Si layers, two-dimensional (2D) metallic states are found to be formed at the interface. From the geometry relaxation, it is shown that the ionic bonding of CuCl is weakened and there is mixed metallic and covalent bonding at the interface. The 2D conduction bands at the interface, sandwiched by the highly polarizable dielectric layers, resemble the 2D Cu-O dpσ bands of the Cu-oxide superconductors, which are considered to be responsible for high T_c superconductivity. To obtain T_c of the CuCl/Si interface based on the conventional electron-phonon(e-p) interactions, we calculated the e-p coupling constant, λ, within the rigid ion approximation [4]. The results indicate that a strong e-p coupling is present at the interface layers but is not enough to explain the previously reported high transition temperature[2].

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