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Longitudinal Phonon Resonance of the Cu(111) Surface VASSE CHIS, BO HELLSING, Department of Physics, Göteborg University, Sweden, MARCO BERNASCONI, GIORGIO BENEDEK, Dipartimento di Scienza dei Materiali, Universita di Milano-Bicocca, Milano, Italy, J. PETER TOENNIES, Max-Planck-Institut fur Dynamik und Selbstorganization, Göttingen, Germany — A density functional perturbation theory investigation of Cu(111) surface dynamics proves that the surface longitudinal acoustic resonance is not an artifact of the inelastic He atom scattering mechanism but a genuine dynamical feature of metal surfaces, and suggests the ability of He atoms to probe the atomic displacements in the second layer through the surface charge modulation they produce. The present results solve the long-standing Bortolani-Mills paradox and reconcile many early apparently divergent interpretations, based on semi-empirical as well as ab-initio methods, of the ubiquitous longitudinal acoustic resonance and clarifies its intrinsic nature.

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