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Crucial electronic contributions to measures of surface diffusion by He atom scattering GUIDO FRATESI, ETSF and Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Milano, IT, GIL ALEXANDROWICZ, Cavendish Laborator, University of Cambridge, Cambridge, UK, MARIO ITALO TRIONI, ETSF and CNISM, UdR Milano-Bicocca, Milano, IT, GIAN PAOLO BRIVIO, ETSF, CNISM, and Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Milano, IT, WILLIAM ALLISON, Cavendish Laboratory, University of Cambridge, Cambridge, UK — In a He atom scattering (HAS) experiment, the position and motion of atoms or molecules at a surface is inferred indirectly, through the electron distribution at the sample surface. Nevertheless, surface diffusion measurements are typically analyzed assuming that the electron distribution simply follows the position of the surface atoms. We have examined theoretically recent HAS measurements of Na/Cu(001), identifying a non trivial relation between the dynamics of the electron distribution and that of the Na ions. The magnitude of the calculated variations in the charge density, and their dependence on the local density of adsorbates, account for the correlated 3D motion experimentally observed. The results of this study further highlight the sensitivity of HAS to the electron distribution of the sample and point out the role of electronic contributions in high-resolution measures of surface dynamics.

Gian Paolo Brivio
ETSF, CNISM, and Dipartimento di Scienza dei Materiali,
Università di Milano-Bicocca, Milano, IT

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