Journal of Physics: Conference Series

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To cite this article: G. A. Bocan *et al* 2017 *J. Phys.: Conf. Ser.* **875** 112002

IOP Conf. Series: Journal of Physics: Conf. Series **875** (2017) 112002 doi:10.1088/1742-6596/875/12/112002

van der Waals effects in GIFAD for light atoms on insulating surfaces

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Synopsis We theoretically address grazing incidence fast atom diffraction (GIFAD) for light atoms on insulating alkali-halide surfaces. We combine a description of the projectile-surface interaction obtained from density functional theory (DFT) calculations with a semiquantum treatment of the dynamics. We obtain simulated intensity profiles and compare them with reported experimental GIFAD patterns. For different systems and incidence conditions we focus on the relevance of van der Waals (vdW) interactions on the diffraction patterns.

Grazing incidence fast atom diffraction (GIFAD) is an extraordinarily sensitive phenomenon. First reported for light atoms on wide band-gap insulating surfaces [1, 2], it has since been observed for a variety of systems, becoming a powerful surface analysis technique as well as a most useful tool for testing potential energy surfaces (PESs).

Achieving an appropriate theoretical description of GIFAD is a challenging task. A projectile-surface potential which includes the key features of the interaction, and a scattering dynamics representation which retains the quantum character of the process are necessary ingredients for attaining good accord with experiments. In this work we accomplish this by combining a description of the projectile-surface interaction by means of a three-dimensional PES, built from high-precision density functional theory calculations; with a semiquantum treatment of the elastic scattering process within the surface initial-value representation (SIVR) [3].

GIFAD theoretical studies that include van der Waals (vdW) interactions are still scarce. However, for certain systems and incidence conditions the role of vdW could be significant. In a recent article, we reported on an important vdW effect on GIFAD for the H/LiF(001) system [4]. It is thus the aim of the present work to further discuss those results and to explore similar systems such as, for example, He/KCl(001) and H/KCl(001).

We consider different systems, incidence channels and perpendicular impact energies. Our results show visible vdW effects on the diffraction patterns provided i) the projectile have a relatively high polarizability, ii) there be no polarization effects along the channel and iii) perpendicular impact energy values be low enough so that the projectile be reflected relatively far from the surface.

These results position GIFAD as a highly sensitive quality check for the various approaches to vdW within DFT, and thus as a promising tool in the development of more accurate descriptions of these interactions.

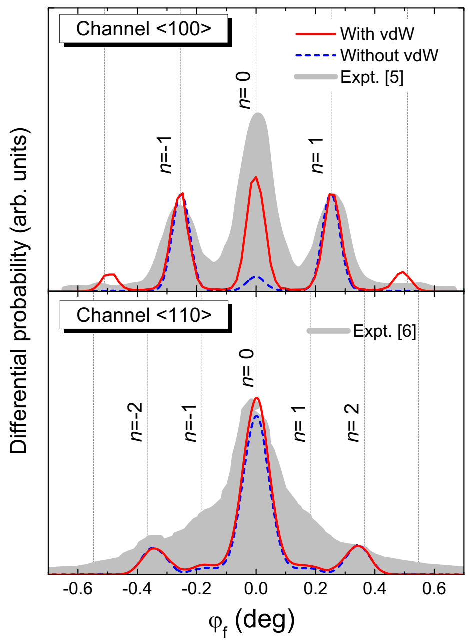

Figure 1. GIFAD for H/LiF(001). Impact energy $E_{tot} = 1$ keV. Incidence angle θ_i relative to surface plane. TOP: $\theta_i = 0.976°$, BOTTOM: $\theta_i = 1.356°$.

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