Exploring the toroidal shape of Holmium and Gadolinium as appearing in qPlus NC-AFM with CO terminated tips

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Single magnetic atoms are important for advancing nanoscale technologies. They are promising for high-density magnetic data storage or quantum computing applications, where stable and controllable magnetic moments are essential. Additionally, in atomic-scale catalysis, the magnetic moment of a single atom can influence reaction pathways, affecting both chemical selectivity and efficiency. Holmium (Ho) and Gadolinium (Gd) are of particular interest due to their large magnetic moments, which make them ideal systems for studying interactions at the atomic scale.

Using non-contact atomic force microscopy (NC-AFM) with a CO functionalized tip, we investigate Ho and Gd adatoms on Cu(111). Constant-height AFM images reveal a toroidal contrast (Figure 1). Previous studies suggest that such features can result from chemical bonding between the adatom and the CO-tip [1] or from probing an anisotropic charge distribution [2]. In the case of chemical bonding, toroidal diameters of approximately 400 pm were reported for Cu and Fe adatoms on Cu(111) [1]. However, in our measurements, we observe significantly larger diameters (~800 pm) for Ho and Gd. Our analysis shows that the toroidal shapes are mainly caused by an electrostatic interaction between the CO terminated tip and the adatoms. A simple electrostatic model successfully reproduces the observed contrast, supporting this interpretation. A similar effect was previously reported in an inversed setup, where a metallic tip scanned CO molecules on different surfaces [3], supporting the idea that electrostatic forces can create toroidal contrast in NC-AFM images.

Additionally, we find that Ho and Gd exclusively adsorb next to substitutional surface defects. When displaced from these defects, the atoms exhibit high mobility, moving readily across the Cu(111) surface. These findings provide new insights into the interplay between magnetic atoms and their local environment, offering potential implications for atomic-scale manipulation and spin-dependent interactions in NC-AFM studies.

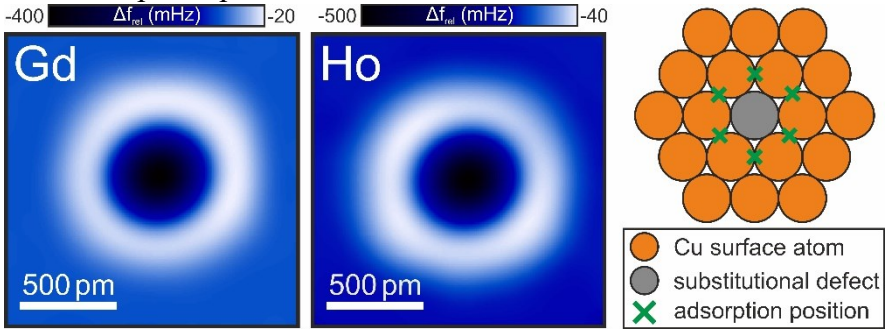

Figure 1. Constant height AFM images of Gadolinium (Gd) and Holmium (Ho) adsorbed on a Cu(111) surface, using a CO terminated tip. The toroidal shape originates form a combination of Van der Waals attraction (dark center) and an electrostatic repulsion (bright ring). Gd and Ho exclusively adsorb right next to substitutional surface defects.

References:

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