Regional chemical potential analysis for atomic force microscopy

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Recently, high-resolution atomic force microscope (AFM) imaging methods that utilize the chemical bonding forces between the AFM probe and material surfaces have been reported for (001) diamond surfaces, and the atomic dimer surface and the ribbons of dimers are identified by AFM experiments and density functional theory (DFT) calculations [1,2]. As the next step, theoretical calculations that enable the quantitative identification and visualization of regions, which are prone to form covalent bonding, are essential for accurately predicting molecular adsorption selectivity and for building a robust theoretical foundation for AFM experiments.

In this study, we theoretically explain that the physical quantity known as the local regional chemical potential (RCP) serves as a measure of electron-donating ability on material surfaces, and we propose that it enables the visualization of chemically active regions such as dangling bonds and double bonds [3]. In other words, the local RCP can serve as an effective measure to interpret high-resolution non-contact or near-contact AFM images enhanced by chemical bonding forces.

To specifically calculate the regional chemical potential $\mu_R^\tau(\vec{r}) = \Delta\varepsilon_\tau(\vec{r})/\Delta n(\vec{r})$ from the electronic states obtained by DFT, we determined the local regional energy density $\Delta\varepsilon_\tau(\vec{r})$ and electron number density $\Delta n(\vec{r})$ within a specified energy range from the Fermi level, and visualized $\mu_R^\tau(\vec{r})$ by plotting it on the zero isosurface of the kinetic energy density representing the material surface. The DFT calculations were performed using OpenMX [4], and post-processing calculations were carried out using the FLPQ module of QEDalpha [5,6]. We will report the electron-donating feature on the surface of the (001) diamond surface.

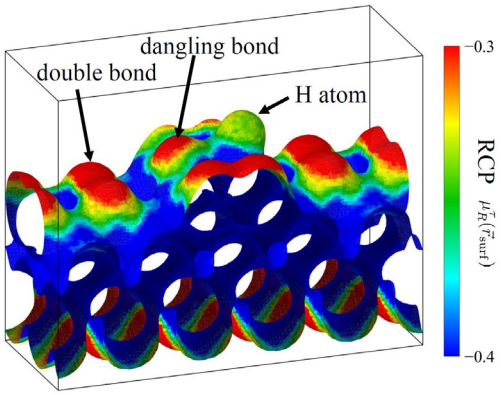

Figure 1. Example of the μ_R distribution on a material surface. The dangling bonds and double bonds in the model of a (001) diamond surface with adsorbed hydrogen atoms are visualized in red.

Reference

[1] R. Zhang, Y. Yasui, M. Fukuda, T. Ozaki, M. Ogura, T. Makino, D. Takeuchi, and Y. Sugimoto, Nano Letters **25**, 1101 (2025).
[2] R. Zhang, Y. Yasui, M. Fukuda, M. Ogura, T. Makino, D. Takeuchi, T. Ozaki, and Y. Sugimoto, Phys. Rev. Res. **7**, 023036 (2025).
[3] M. Fukuda, M. Senami, Y. Sugimoto, and T. Ozaki, arXiv:2505.04053.
[4] OpenMX, http://www.openmx-square.org/.
[5] QEDalpha, https://github.com/mfukudaQED/QEDalpha.
[6] FLPQ module in QEDalpha, https://github.com/mfukudaQED/FLPQ.