

## Publication

## Reconstruction of a 2D layer of KBr on Ir(111) and electromechanical alteration by graphene

**JournalArticle (Originalarbeit in einer wissenschaftlichen Zeitschrift)****ID** 4638160**Author(s)** Liu, Zhao; Hinaut, Antoine; Peeters, Stefan; Scherb, Sebastian; Meyer, Ernst; Righi, Maria Clelia; Glatzel, Thilo**Author(s) at UniBasel** [Glatzel, Thilo](#) ; [Meyer, Ernst](#) ; [Hinaut, Antoine](#) ;**Year** 2021**Title** Reconstruction of a 2D layer of KBr on Ir(111) and electromechanical alteration by graphene**Journal** Beilstein Journal of Nanotechnology**Volume** 12**Pages / Article-Number** 432-439**Keywords** DFT; Ir(111); KBr; KPFM; graphene; nc-AFM; surface reconstruction

A novel reconstruction of a two-dimensional layer of KBr on an Ir(111) surface is observed by high-resolution noncontact atomic force microscopy and verified by density functional theory (DFT). The observed KBr structure is oriented along the main directions of the Ir(111) surface, but forms a characteristic double-line pattern. Comprehensive calculations by DFT, taking into account the observed periodicities, resulted in a new low-energy reconstruction. However, it is fully relaxed into a common cubic structure when a monolayer of graphene is located between substrate and KBr. By using Kelvin probe force microscopy, the work functions of the reconstructed and the cubic configuration of KBr were measured and indicate, in accordance with the DFT calculations, a difference of nearly 900 meV. The difference is due to the strong interaction and local charge displacement of the K; +; /Br; -; ions and the Ir(111) surface, which are reduced by the decoupling effect of graphene, thus yielding different electrical and mechanical properties of the top KBr layer.

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