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Supporting Information

for

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

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Additional experimental data

After additional calculations, the cell that remains most representative contains 12 Ir and 7 KBr units along the x direction (horizontal direction in the slides). Indeed the mismatch between the theoretical lattice parameters of KBr and Ir within this cell (-1.98%) is very similar to the experimental one of -1.86% in the cell containing 21 Ir units. Moreover, the energy of the relaxed structure in this cell is the lowest among all considered. So we may refer to this structure for a possible model of the "local" system geometry and partial charges.

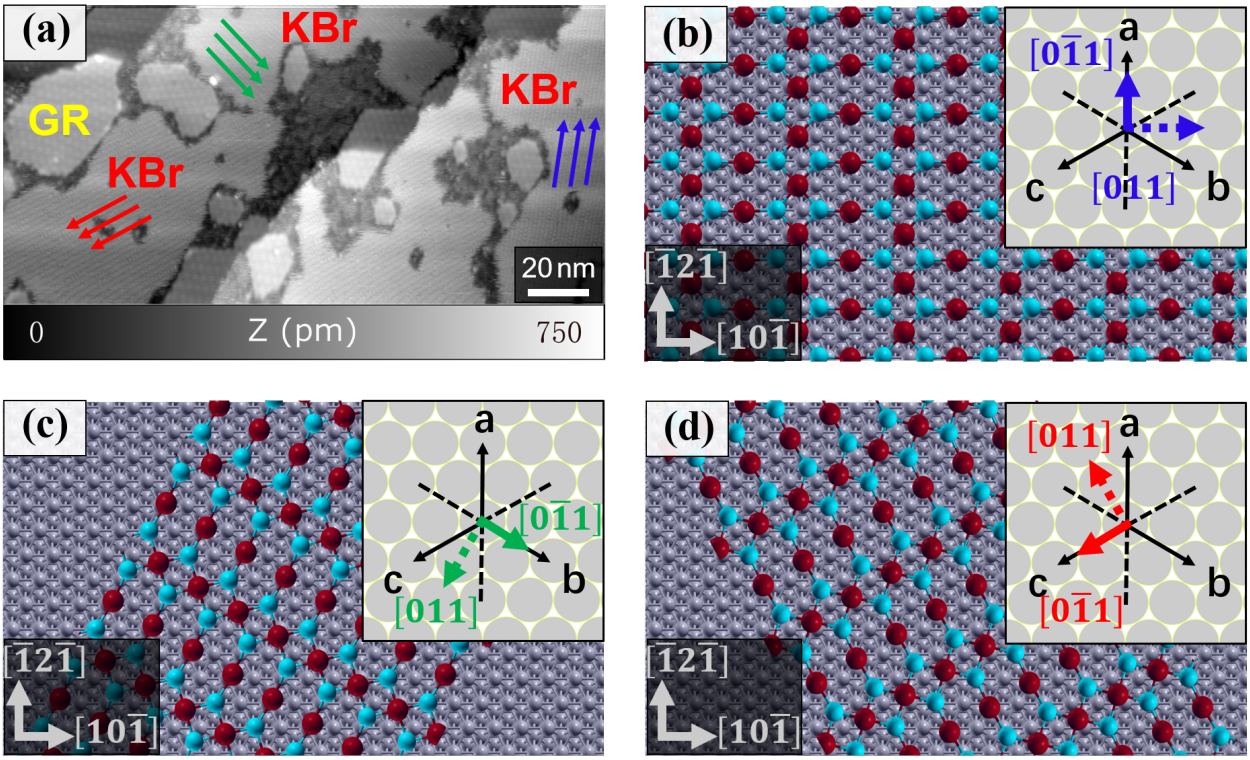

Figure S1: Three rotated domains of the reconstructed KBr(100) lattice with the related models (inset orthogonal arrows with the solid line for [0$\bar{1}$1] (orientation without corrugation) and dotted line for [011] (orientation with corrugation) on hexagonal Ir(111) surface (red for Br atoms, blue for K atoms and grey for iridium atoms)). (a) Topography image of three KBr orientations on Ir(111) in total via nc-AFM ($A_1 = 2\,\mathrm{nm}$, $\Delta f_1 = -30\,\mathrm{Hz}$, $\gamma = -25.9\,\mathrm{pN\,nm}^{1/2}$). (b) Model in 0° rotation. (c) Model in 120° rotation. (d) Model in −120° rotation.

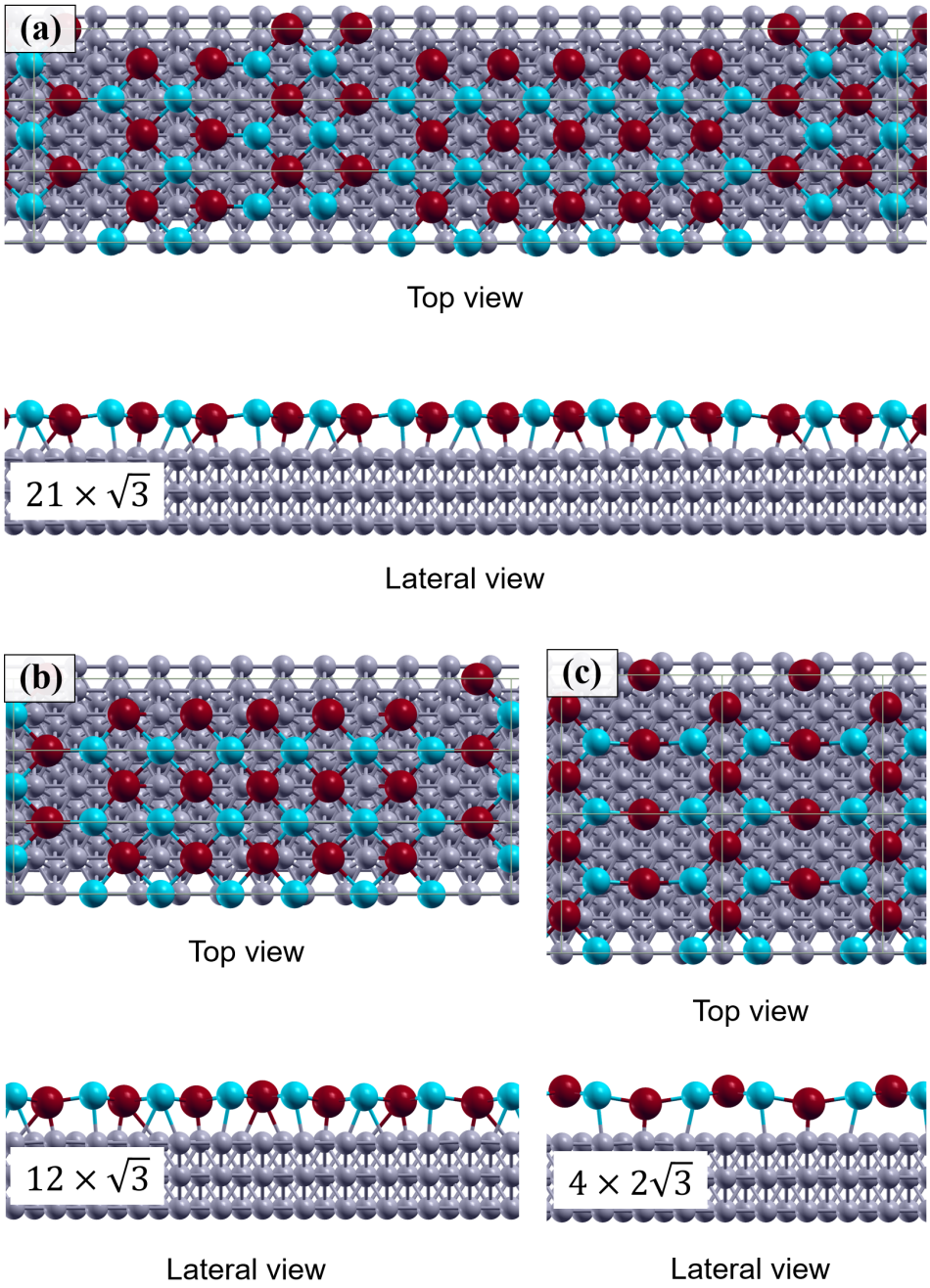

Figure S2: Three calculated KBr reconstructed models on Ir(111) by DFT method from long to short periodicities (red for Br atoms, blue for K atoms and grey for iridium atoms). (a) 21 $\times\sqrt{3}$, repeated three times along the $[0\bar{1}1]$ direction, with the adsorption energy of -0.46 eV/unit. (b) 12 $\times\sqrt{3}$, repeated three times along the $[0\bar{1}1]$ direction, with the adsorption energy of -0.82 eV/unit. (c) 4 $\times 2\sqrt{3}$, repeated two times along the $[0\bar{1}1]$ direction, with the adsorption energy of -0.91 eV/unit.

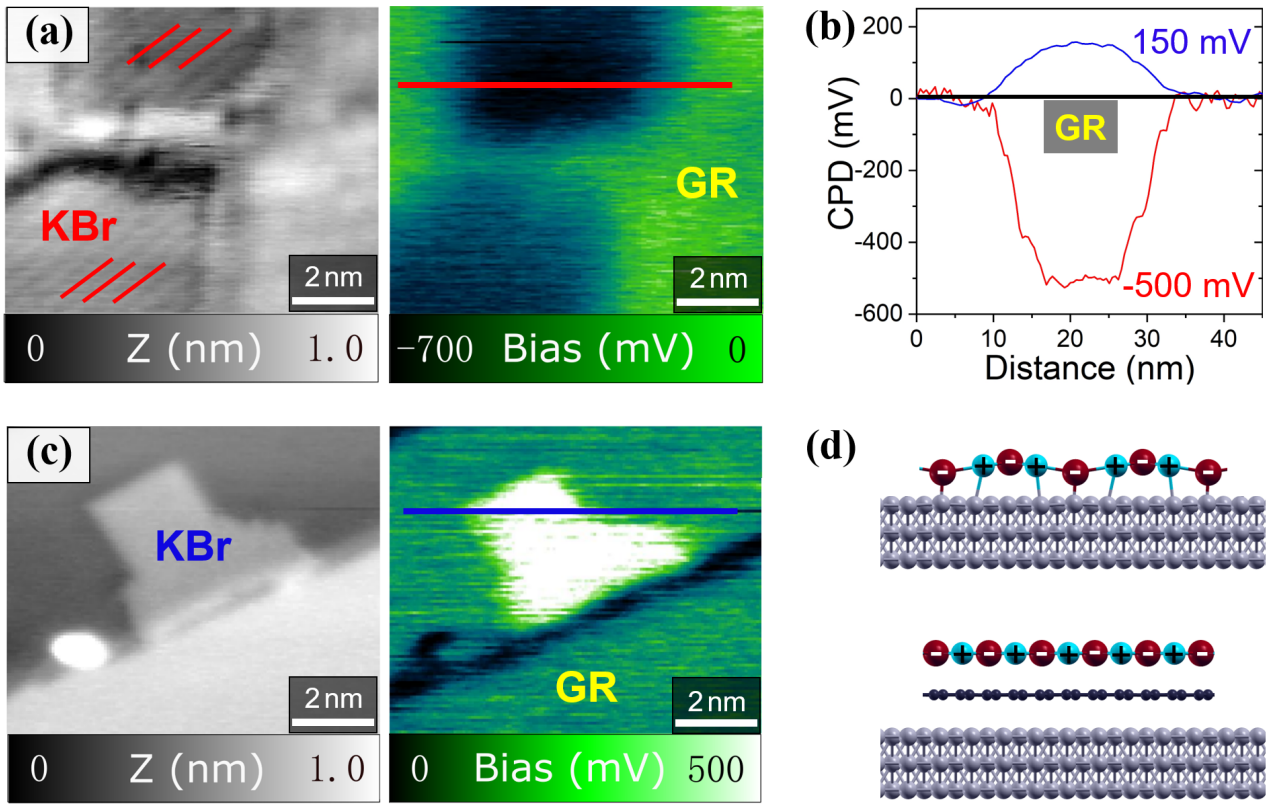

Figure S3: KPFM images of KBr islands accompanied with topography in nc-AFM. (a) KBr island next to the graphene flake ($A_1 = 2\,\text{nm}$, $\Delta f_1 = -15\,\text{Hz}$, $\gamma = -12.9\,\text{pN}\,\text{nm}^{1/2}$). (b) CPD profiles of two KBr in (a) and (c) compared with graphene. (c) KBr island on the graphene sheet ($A_1 = 5\,\text{nm}$, $\Delta f_1 = -5\,\text{Hz}$, $\gamma = -17.1\,\text{pN}\,\text{nm}^{1/2}$). (d) The separated charge layers in the reconstructed KBr and the electrically neutral state in the cubic KBr (red for Br atom, blue for K atom and grey for iridium atom).