Moiré-trapped polarons in the type-II multiferroic $NiBr_2$ monolayers

Valeria SHEINA[1], Emmanuel CALDERON[1], Arindam MUKHERJEE[1], Hugo LE DU[1], Robin SALVATORE[1], François DEBONDRIDDER[1], Marie D'ANGELO[1], Tristan CREN[1], Marie HERVE[1]

[1]Sorbonne Université – CNRS - Institut des Nanosciences de Paris UMR7588, 4 place Jussieu, Paris 75005, France

Transition metal dihalides (TMDHs) constitute a class of van der Waals materials exhibiting rich magnetic phase diagrams, making them promising candidates for next-generation spintronic and magnetoelectric applications [1-5]. In the bulk $NiBr_2$ displays in-plane ferromagnetic ordering with antiferromagnetic interlayer coupling [1]. At low temperatures, competing exchange interactions and magnetic frustration stabilize a non-collinear helimagnetic ground state, accompanied by Type-II multiferroicity [1,2,4]. In the monolayer limit, these magnetic and electronic properties could be strongly modified by substrate-induced effects, including strain, chemical alternation, and charge transfer [3,4].

In addition, a monolayer TMDHs can host intrinsic polarons—composite quasiparticles formed when an excess charge carrier is localized by self-induced lattice distortions. Unlike historically studied polarons pinned to extrinsic defects, these intrinsic states emerge in defect-less lattices through a cooperative interplay between electron-phonon coupling and electron-electron interactions [5].

In this work, we utilize low-temperature scanning tunneling microscopy and spectroscopy to investigate the electronic and magnetic properties of monolayer $NiBr_2$ grown epitaxially on Au(111) and HOPG. Our findings highlight three key observations. First, we resolve a Moiré superlattice arising from the lattice mismatch between the $NiBr_2$ film and the underlying substrates (Fig.1 a and b). Second, on the Au(111) substrate, we identify a high density of intrinsic small polarons characterized by narrow in-gap electronic states. By applying high-bias voltage pulses, we demonstrate the atomic-scale manipulation of individual polarons, revealing that their site-to-site hopping and lateral dynamics are strictly governed by the Moiré pinning sites. Finally, we resolve multiferroic spin-spiral contrast exclusively on the HOPG substrate (Fig.1 b), while this order remains absent in STM measurements on the metallic Au(111) interface. These results establish the $NiBr_2$ interface as a robust platform for the atomic-scale engineering of localized charge density and magnetoelectric phases.

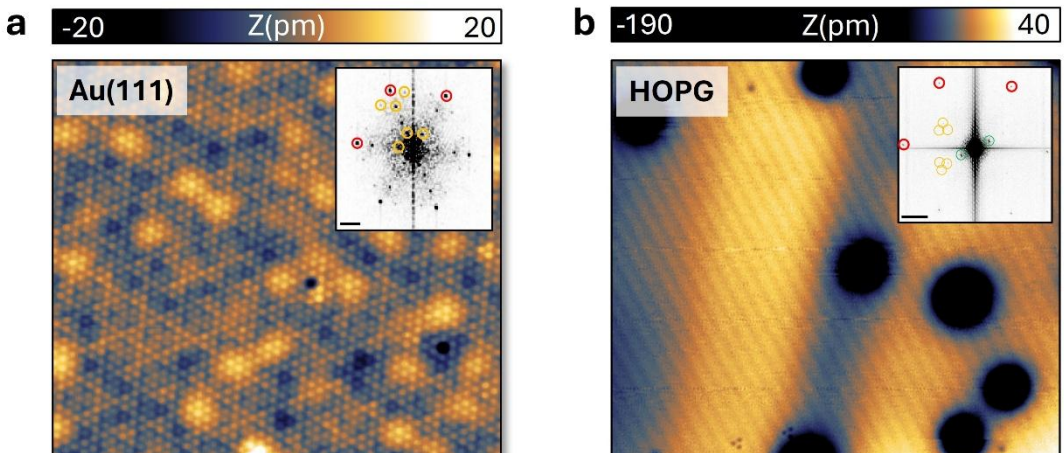

Figure 1 a. STM topography of 1ML $NiBr_2$/Au(111) (V_{bias} = *0.2 V*, I_{set} = *100 pA, T = 4.2 K*). b. STM topography of 1ML $NiBr_2$/HOPG (V_{bias} = *0.7 V*, I_{set} = *100 pA, T = 3 K*). Both: Scale bare : 10nm. Inset : 2D FFT with scale bare of 1 nm^{-1}.

REFERENCES

1. Botana, A. S. et al. Phys rev materials **2019**, 3, 044001
2. Cahlík, A. et al. arXiv **2026**, 2601.20713v1
3. Miao, M.-P.; et al. PNAS **2025** , 122, 29
4. Bikaljević, D. et al. ACS Nano **2021**, 15/9, 14985
5. Cai, M. et al. Nat Commun **2023**, 14, 3691