The Carbon Radical Ion (CRI) in Monolayer WS_2

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2D materials are an exciting host to engineer atomic quantum systems by chemical design principles. In this talk, I will give a brief overview on our efforts to design defect systems in monolayer transition metal dichalcogenides (TMDs) by means of chemical doping, He ion beam bombardment and atomic manipulation. Individual point defects in such samples were studied by means of high-resolution scanning probe microscopy. [1-7]

In particular, we demonstrate the atomically controlled generation of magnetic carbon radical ions (CRIs) in synthetic TMDs [8]. First, carbon-hydrogen impurities were introduced into TMDs by a post-synthetic methane plasma treatment [6]. These CH impurities are negatively charged and hence exhibit a series of hydrogenic bound and resonant states emerging from different valence band maxima [4]. Interestingly, the carbon-hydrogen impurities can be activated by tip-induced hydrogen desorption with atomic precision [8]. The resulting dangling bond can be charged and decharged by the underlying graphene substrate. In its anionic state, the carbon impurity exhibits an out-of-plane magnetic moment of $1\mu_B$ resulting from a half-occupied deep in-gap orbital. We also quantify the full vibronic response of the TMD lattice to the defect ionization, which exhibits a striking dependence on the charge polarity and number of TMD layers.

References:

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