

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Carrier injection in van der Waals multilayer systems MARCELO KURODA, CHRISTOPHER COGER, Auburn University — Carrier injection is critical for the use of two-dimensional material systems like transition metal dichalcogenides (TMD) or graphene in electronic devices. Here we use first principles calculations (within the density functional theory) to quantify and classify the contact formed between metals and TMD multilayer systems. In particular we study the cases of multilayer MoS₂ and MoSe₂ with different metal electrodes (e.g. Pd, Au, Ti). We find different behaviors depending on the choice of metal, thickness and electric field. An analytical model is produced accounting for the Fermi level pinning and the layer quantum capacitance. This atomistic description also sheds light on the ambipolar behavior observed in these systems and the gate-dependent contact resistance in field effect transistors.

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Date submitted: 14 Nov 2014

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