

Theoretical and Experimental Observation of Anisotropic 2D Excitons in Self-Assembled Hybrid Quantum Wells

Lorenzo Maserati

(Nanofabrication Facility – Affiliate, The Molecular Foundry - Lawrence Berkeley National Laboratory

Printed and Molecular Electronic Group – Researcher, Center for Nano Science and Technology – Istituto Italiano di Tecnologia)

Self-assembled metal organic materials have great potential for optoelectronic applications due to their atomic and structural tunability. While a vast library of these materials has been studied, understanding optoelectronic properties to drive synthesis has been nearly impossible due to their complex structure. Here we consider the self-assembled layered bulk silver benzeneselenolate, $[\text{AgSePh}]_{\infty}$, as a representative of a class of coordination polymers exhibiting quantum well characteristics. Using ab initio density functional theory (DFT) and GW and Bethe-Salpeter equation (BSE) approach calculations, we predict and experimentally confirm two-dimensional (2D)-like excitonic and optoelectronic properties in the bulk phase arising from the quantum-confined charge carriers, including large exciton binding energies (~380 meV) and anisotropic absorption and emission. Our study demonstrates how integrating theory and experiment can elucidate general features in hybrid chalcogenide materials scalable *via* supramolecular chemistry with strong excitonic effects in the presence of anisotropic screening and strong confinement.

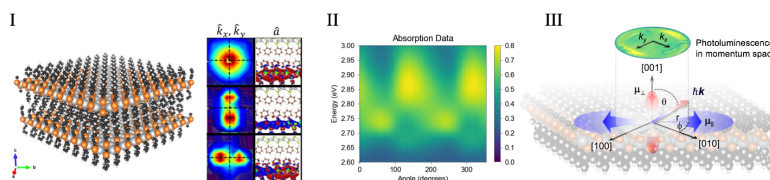


Figure 1. I, Material molecular representation with visualization of the predicted excitonic resonances. II, Experimentally measured strong absorption anisotropy. III, Experimentally observed anisotropic excitonic photoluminescence



Lorenzo Maserati Dr. Lorenzo Maserati graduated from Politecnico di Milano with a BSc (2007) and MSc (2009) in Physics Engineering. He obtained his PhD in Nanosciences from University of Genoa (IIT, 2014) with a thesis on colloidal nanocrystal films for optoelectronic applications. Then he joined the Lawrence Berkeley National Lab (LBNL) where he developed metal-organic frameworks membranes for gas separation. In a second postdoctoral appointment at LBNL, he focused his work on the excitonic properties of 2D and 2D-like materials, investigated by ultrafast spectroscopy. Dr. Maserati is currently Researcher at CNST (IIT) in Milan where he studies self-assembled metal-organic chalcogenides for optoelectronic applications. His interests range from materials chemistry to solid state and device physics. He is recipient of the “NanoInnovators’s got talent” award (Rome, 2016), and the Marie-Curie Seal of Excellence (2017).

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