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Abstract for an Invited Paper
for the MAR13 Meeting of
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Tuning charge transport in organic devices: From in silico to carbon to device

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I will describe our work towards first-principles design of organic semiconducting materials. In particular, I will describe our efforts towards the rational design of high hole-mobility organic crystals. I will describe a case study where the in silico prediction of a material led to the synthesis and characterization of it by the Bao and Toney groups. I will also discuss other related research directions.