RFR Model, Charge Transition Levels (eV) **Training** Test CdTe<sub>0.5</sub>Se<sub>0.5</sub> ML Prediction CdSe<sub>0.5</sub>S<sub>0.5</sub> Out rmse = 0.35 eV Test rmse = 0.34 eV Train rmse = 0.20 eV **DFT Calculation**