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Designing Semiconductor Heterostructures Using Digitally Accessible Electronic-Structure Data ETHAN SHAPERA, Department of Physics, UIUC, ANDRE SCHLEIFE, Department of Materials Science and Engineering, UIUC — Semiconductor sandwich structures, so-called heterojunctions, are at the heart of modern applications with tremendous societal impact: Light-emitting diodes shape the future of lighting and solar cells are promising for renewable energy. However, their computer-based design is hampered by the high cost of electronic structure techniques used to select materials based on alignment of valence and conduction bands and to evaluate excited state properties. We describe, validate, and demonstrate an open source Python framework which rapidly screens existing online databases and user-provided data to find combinations of suitable, previously fabricated materials for optoelectronic applications. The branch point energy aligns valence and conduction bands of different materials, requiring only the bulk density functional theory band structure. We train machine learning algorithms to predict the dielectric constant, electron mobility, and hole mobility with material descriptors available in online databases. Using CdSe and InP as emitting layers for LEDs and $CH_3NH_3PbI_3$ and nanoparticle PbS as absorbers for solar cells, we demonstrate our broadly applicable, automated method.

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