Theoretical models of Amorphous Oxides

1. ~~**Classical Molecular Dynamics:** cannot capture defect/localized states…~~
2. **Ab-initio Molecular Dynamics:** solves DFT equations for each MD step

MD liquid-quench simulations

- Crystal melted at 3000K
- Cycles of quenching at K/ps rate
- Relaxed at 300K
- DFT optimization for electronic and optical properties

Outcome

- Structure of 1st, 2nd, 3rd shells
- MO_x spatial distribution
- Shallow, deep, trap defects
- Role of cooling rate, composition, oxygen stoichiometry
- Structural, electronic, optical, transport, mechanical properties