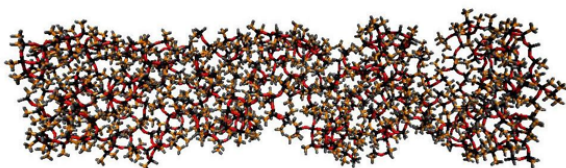


Clancy group: 2016 PhD projects– Electronic materials

1. Reactive Force Field Design of Coatings on Glassy Materials (Herbol, Reveil)



- How best to model a reactive system involving coatings on glass?
- Collaboration with Corning
- How to model “large” systems of reactive atoms that form HOIPs?
- Collaboration with Estroff group

NEW

- *Algorithm development*
- Reactive force field capable of making- and breaking- chemical bonds
- Proof-of-concept published in 2016 for PbSe quantum dots
- But systems like glasses or hybrid organic-inorganic perovskites require more complex directional forces
- *Requires good computational skills*