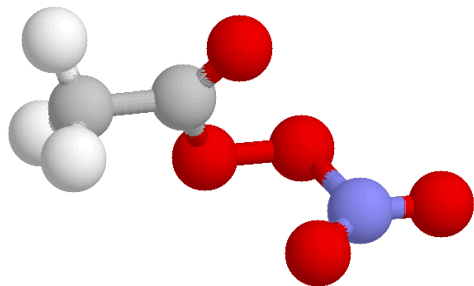
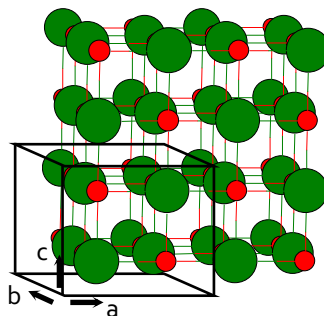


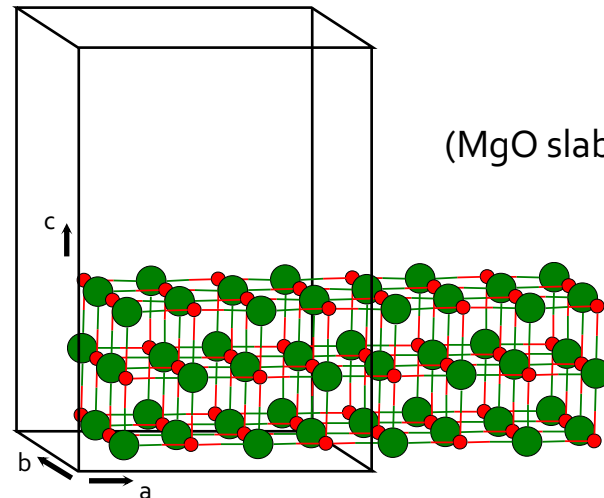
(peroxyacetyl nitrate)



(MgO bulk)



(MgO slab)



“cluster” models

Isolated molecule in vacuum
(or dielectric continuum)

Gas-phase

Solution-phase

“Localized” chemistry

Amenable to highly
accurate calculations

“supercell” models

3-D periodic boundary conditions applied to atomic
configuration

Bulk solids

Bulk liquids

Surfaces and Interfaces

“Delocalized” chemistry

Amenable to highly efficient calculations