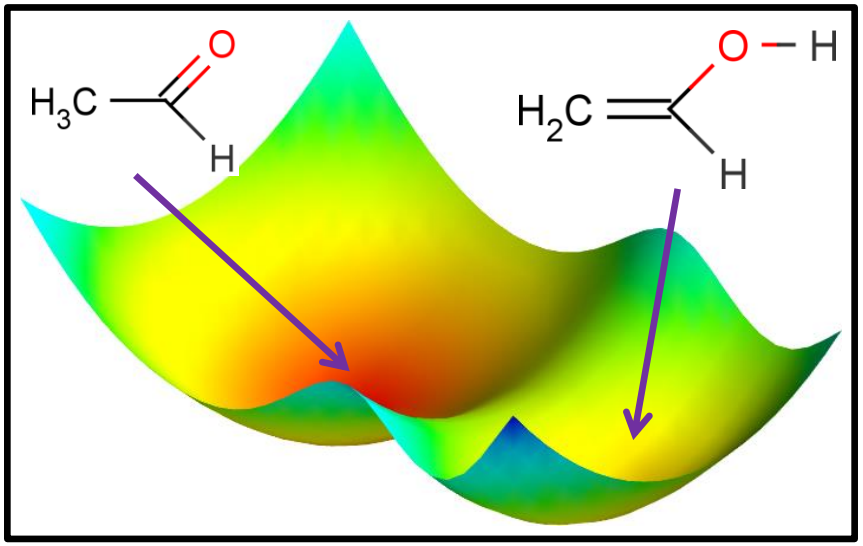
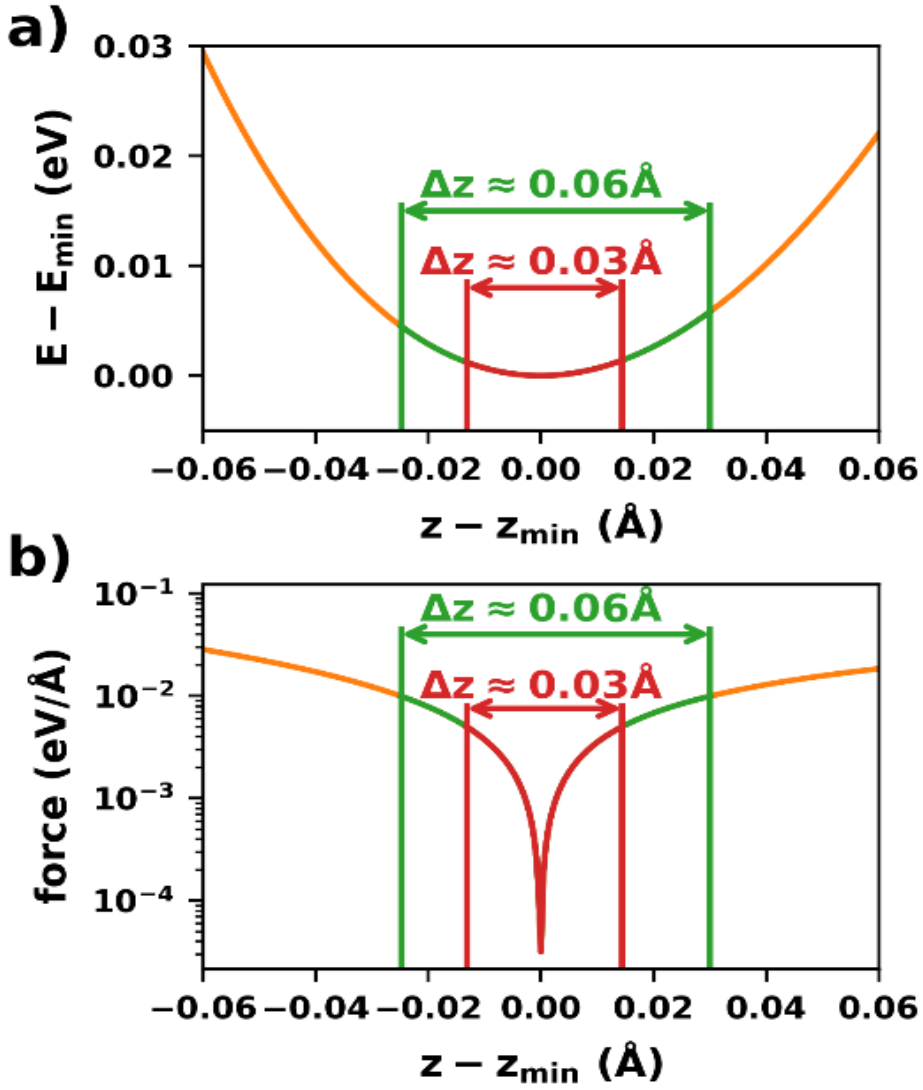
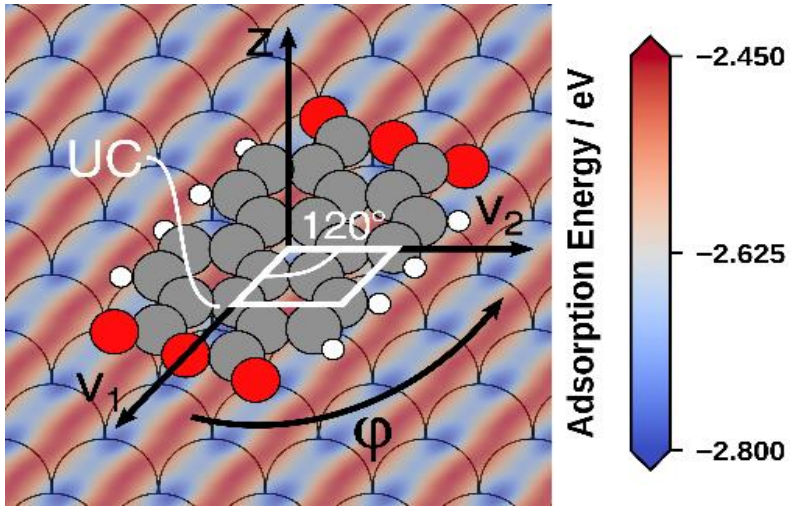
# Applications of Electronic Structure Methods

## Tips

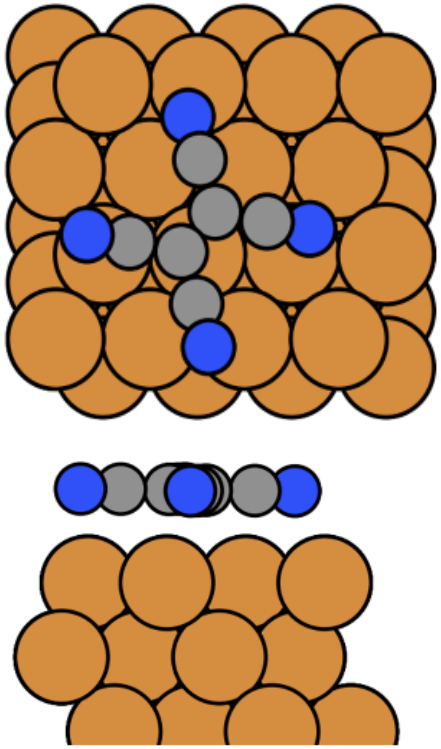


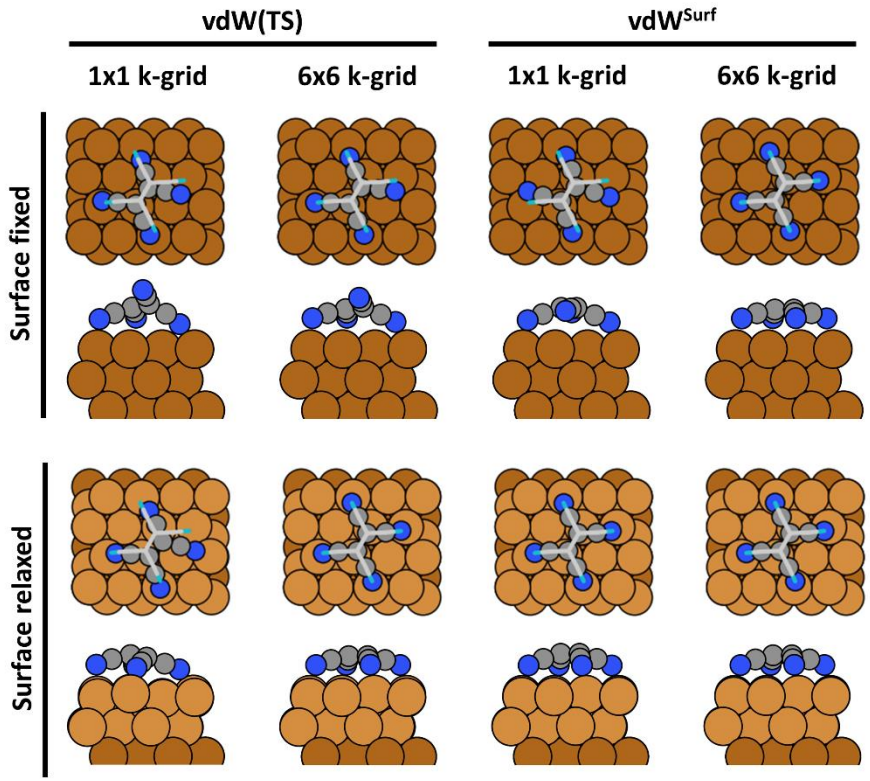
# How Accurate is the Geometry?



# Cutting Corners

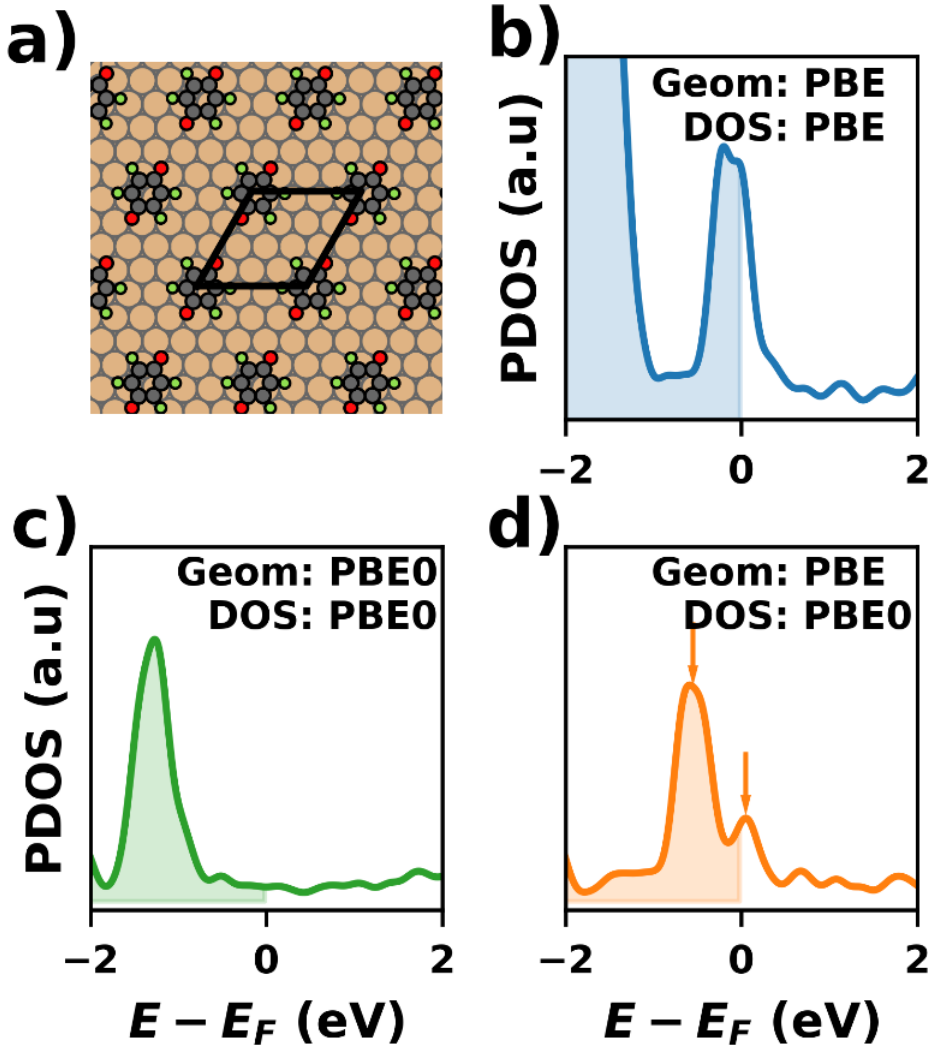





**Potential to speed up calculations (fewer DOFs)**

**May create artificial minima**

# Consistency of Electronic and Geometric Structure



# Conclusions

## Local geometry optimization: Follow gradient

- Hellman-Feynman from moving potentials
- Pulay from moving basis functions
- + additional terms

## Quasi-Newton method *de-facto* standard

- Require approximation and update of Hessian
- Step control by line search or trust radius method
- Works best near minimum

**Recommended procedure: Pre-relax with Conjugate Gradient (get close to minimum), finish with Quasi-Newton method**

# Self-assessment

**https://fbr.io/join/twbyw**