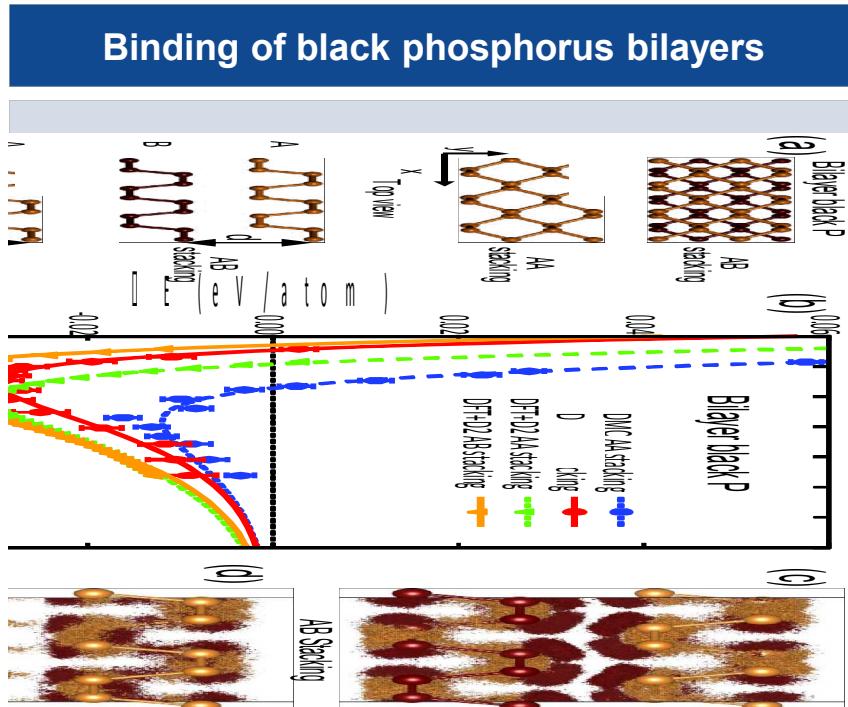


Tracking# (SAND, PR) _____

- Van der Waals interactions between closed shell molecules are notoriously difficult to treat consistently with ab initio methods
- Focus on layered black phosphorus
- Showed that interactions between layers are more complex than a simple dispersion interaction
- Significant reorganization of electrons due to presence of nearby layers
- Study lays the groundwork for future calculations on explosive crystals

Principal Investigator: L. Shulenburger
 Platform and Campaign ID: Sequoia – CCC7-124
 Usage: 2.07 Days



The binding of bilayers of black phosphorus is significantly affected by the orientation of the layers. The panels on the right show significant charge reorganization due to the interaction (red is depletion of electron density, red is enhancement)