US-Africa Initiative Workshop

APS March Meeting - Sunday, March 14, 2021

Sponsored by the APS Innovation Fund

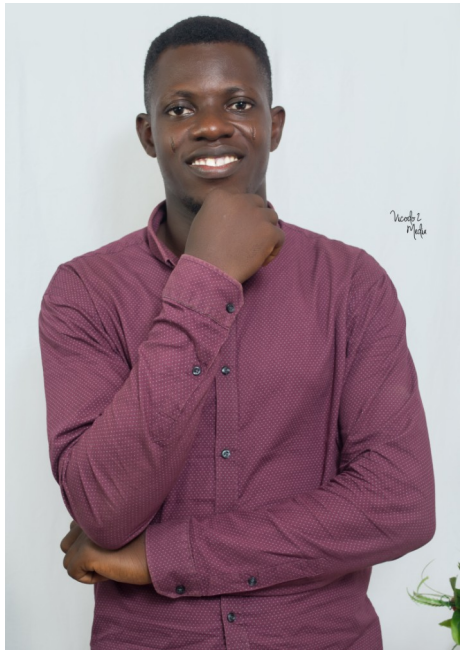
[Omololu AKIN-OJO]

ICTP East African Institute for Fundamental Research (EAIFR), Rwanda

Major interest is in "Methods Development": Accurate results "without too much computation" includes force field development, Improved Tight Binding /Semi-Empirical methods from ab initio data and now, Machine Learning

Secondary interest is in the application of these methods *to technologically important systems and, possibly biomedical applications*

Ezekiel Oyeniyi, PhD Candidate Univ. Ibadan: EOMCCSD -> ZINDO/S



Damilare Babatunde, MSc Candidate Univ. Ibadan: Water Splitting

Akorede Joledo, PhD Candidate Univ. Ibadan: Water Splitting

Firas Shuaib, MSc Graduate, Univ. Rwanda ML in Superconductivity

Sosthene Irambona, PhD Candidate Univ. Rwanda DFT+U

Ayoola Adeolu, PhD Candidate Univ. Ibadan: Battery Research

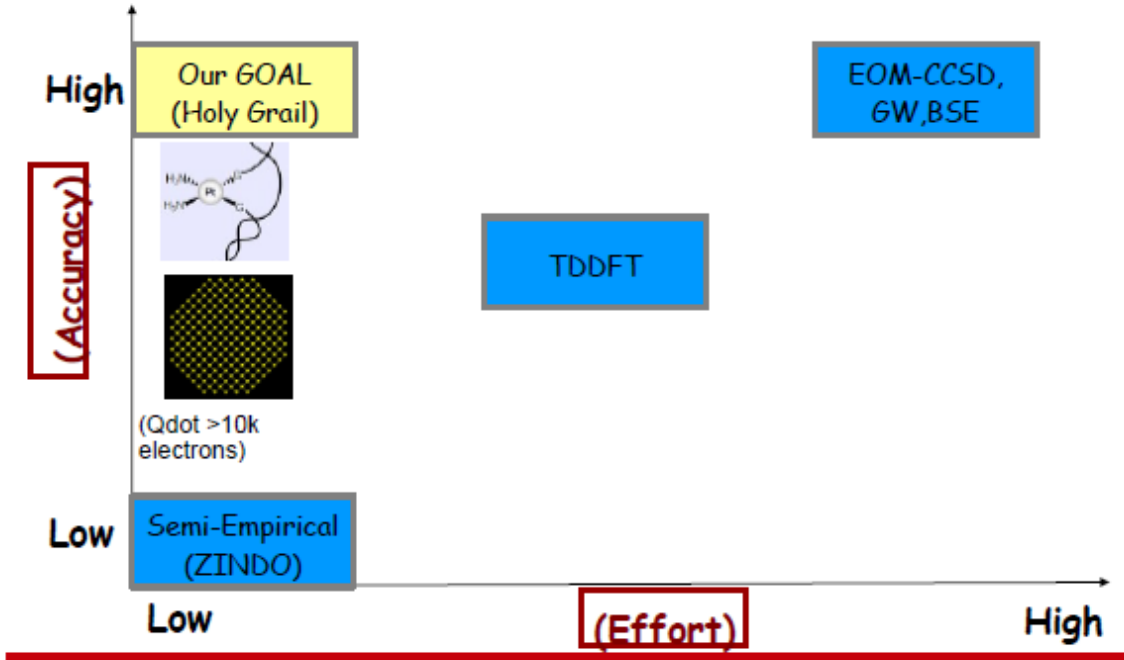
[Research Efforts and Collaborations in Akin-Ojo Research Group at EAIFR]

- Excited States for large systems: Second-Principles methods giving near-EOM-CCSD results at ZINDO/S cost
- Strongly Correlated Systems – DFT+U from atoms to compounds
- Predicting Superconducting Materials from Machine Learning
- Photocatalytic Water Splitting: Investigating SiNi, CNi, Si_2FeZn on MgO support for water splitting
- Battery research (beginning) using xTB and semi-empirical methods in MD
- Bulk Modulus of Osmium nanostructures
- Orbital-Free DFT (OFDFT): Search for Kinetic Energy Density Functional

[Example]

A second-principles approach for efficient determination of excitation energies and absorption spectra of quantum dots and large systems from ab initio data

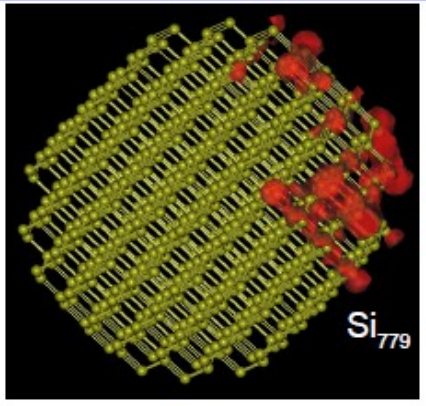
... approximate practical methods of applying quantum mechanics ... [to explain] main features of complex atomic systems without too much computation – PAM Dirac, 1929

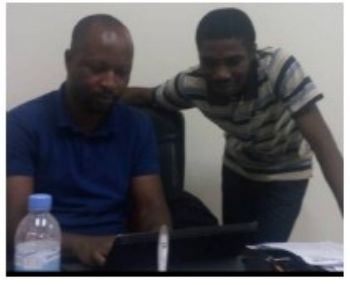


→ Fast + Accurate Prediction of Material Properties

EOM-CCSD → "oeINDO" : DIATOMIC

Si_{779}
10,906 electrons
3,116 valence electrons
21-hr calculation on 1 processor





RESULTS: Mean Absolute Error (MAE): 0.2 eV

Methods	EOM-CCSD	TDDFT	CIS(D)
Si_3			
oeINDO	0.22	0.17	0.39
ZINDO/S	0.91	0.98	0.74
Si_4			
oeINDO	0.18	0.24	0.31
ZINDO/S	1.38	1.71	1.25
Si_5			
oeINDO	0.09	0.04	0.16
ZINDO/S	1.47	1.52	1.39
Si_{19}			
oeINDO	-	0.32	0.36
ZINDO/S	-	1.42	1.46
Si_{40}			
oeINDO	-	0.12	0.03
ZINDO/S	-	0.68	0.80