Quantum Mechanics Floes in Orion: It's not just for CSP anymore! Caitlin C. Bannan Scientific Developer II, Physics Group CUP XXI





"I can do things you cannot, you can do things I cannot; together we can do great things." – Mother Teresa

Photo Credit: BBC

Core

technology

platform

Third-Party Scientific Methods









Floes integrate toolkits, QM, and custom analysis



Torsion Scanning

- Select one single bond
- Scan all rotatable bonds
- Generate custom Omega rules

Conformer Analysis

- Diverse ensemble
- Local minima search
- Compare tautomers





Compare energy distributions for both tautomers





penEue

Gas phase QM calculations make CSP possible



Later today: "CSP is Difficult, but not Impossible!"

- Hari Muddana









Spectra Predictions





9 Molecule and Spectra created in GaussView, rxn coordinate: https://www.scm.com/doc/Tutorials/StructureAndReactivity/ZN-PES-Scan_TST.html

Method	Pros	Cons



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Run Gaussian input files with Orion as a computational engine		



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Input

- Gaussian input file (.com/.gjf)
- Many saved in a Tar or Zip file

Output

- Tar file saving output
- Sub-directory/calculation



Calculate HOMO-LUMO Gap: GaussView and Orion







22 atoms, 90 electrons, neutral, singlet, C12H9F







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Integrate Gaussian calculations with datasets









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Thank You

Please share your dream properties and example input files!

