Introduction to Entos:
Quantum Chemical Simulation Software

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Entos enables *ab initio* simulation of molecular and condensed-phase chemical reactions and other processes, with particular focus on mean-field (i.e., DFT), quantum embedding methods, and physics-based machine-learning for electronic structure. The software has proven successful for the simulation of systems ranging across homogenous catalysis, heterogeneous catalysis, and solvent properties and design, and it is a powerful tool for generating features for machine-learning applications. Entos is built to easily integrate with research workflows, allowing integration via simple text I/O, JSON output, and interactive Jupyter notebooks.

Prerequisites: Basic electronic structure methods for chemistry/materials; Basic Unix/Linux, Python, or Jupyter notebook skills.

The tutorial will focus on topics that include:

- Geometry optimizations
- transition-state searches
- implicit and explicit (QM/MM) solvation
- electronically excited states
- NMR and other spectroscopic properties
- Conformer search methods
- Molecular dynamics
- Quantum embedding (embedded mean-field theory)

The course will include demonstrations and a cloud-based interactive tutorial (jupyter.entos.ai).

Note: To participate in any live demonstrations, please obtain a Github account.
Attendees are welcome to follow the zoom presentation, even without a Github account.

Additional information about Entos can be found at:

www.entos.ai