University of New Haven

PhD Positions in AI-Driven Catalyst Design at the University of New Haven, USA

The Center of Integrative Materials Discovery (the IMD Center) at the University of New Haven (West Haven, CT, the United States) has two openings for PhD students in AI-driven catalyst design for biomass conversion or CO_2 conversion, for the admission of Fall 2023. The IMD Center led by Prof. Dequan Xiao (associate professor in chemistry, Department of Chemistry and Chemical and Biomedical Engineering) is focused on developing and integrating theoretical & computational chemistry methods with experimental methods to drive the discovery of novel chemicals, such as catalysts, polymers, and molecular drugs. More details about can be found at the IMD Center website.

Here are three basic requirements for the PhD position.
1. The candidate should hold a BS or MS degree in chemistry or related areas.
2. The candidate should have research interests in theoretical/computational chemistry and developing AI-driven methods for catalyst design.
3. The candidate should have sufficient English proficiency for the purpose of conducting research and publishing papers.

The research projects may include the following skills/tasks. Any previous learning or research experience related to these skills will be helpful but not required for the PhD candidate.
1. Perform quantum chemistry analysis for catalytic mechanisms using density functional theory.
2. Perform catalyst design using inverse molecular design theory and/or AI driven approaches.
3. Study the catalytic reactions for biomass conversion and/or CO_2 conversion.
4. Publish research results in peer-reviewed journals.
5. Collaborate with other researchers within or outside the institution.
6. Perform experimental catalysis. This is optional.
Either domestic or international students are welcome to apply for these positions.

The details of applying for the PhD positions can be found by the following link.
https://www.newhaven.edu/engineering/graduate-programs/engineering-applied-science-phd/index.php

Note: The University of New Haven is a private, top-tier comprehensive institution recognized as a national leader in experiential education. Founded in 1920 on the campus of Yale University in cooperation with Northeastern University, UNH moved to its current West Haven campus in 1960. The University provides its students with a unique combination of a solid liberal arts education and real-world, hands-on career and research opportunities. UNH enrolls approximately 7,513, including nearly 2,490 graduate students and 5,023 undergraduates – the majority of whom reside in University housing.