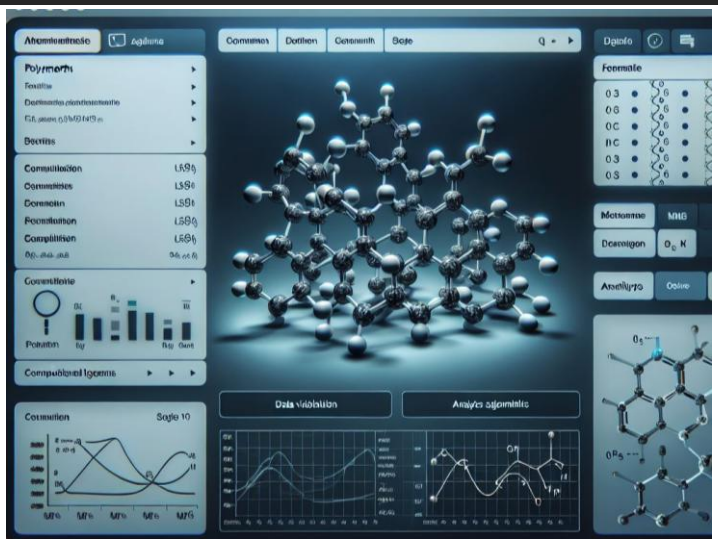
NovaUCD

Technology Licensing Opportunity

Crystal structure prediction

Novel technology to accelerate screening in new material discovery



Opportunity

Crystal structure prediction plays a critical role in materials science and condensed matter physics, as it enables researchers to theoretically assess and design new materials with desirable properties. However, accurately simulating material behaviour remains challenging due to the intrinsic complexity of interactions in condensed systems, where small unit cells and periodic boundary conditions restrict the fidelity of conventional energy calculations. Conventional approaches are hampered by limitations that stem from their handling of non-electrostatic interactions and the narrow confines imposed by simulation cell boundaries.

Technology Overview

This invention uses a supercell approach with basin-hopping optimization to efficiently calculate configurational energy in crystal structure prediction, overcoming size limitations and accurately handling diverse energy interactions for various complex molecular systems.

Key Features/Advantages:

•Enables calculation with a larger cutoff radius via a supercell approach, improving energy accuracy without extra computational cost.

•Integrates with a basin-hopping optimization algorithm to efficiently locate global minimum enthalpy configurations.

•Accurately handles complex systems by incorporating intramolecular energy and allowing dynamic supercell adjustments.

Value Proposition:
Novel way to screen materials to identify the most stable form

Markets:
Battery materials simulation
High-throughput materials discovery
Molecular crystal design

Lead Inventors:
Professor Niall English

IP Status/Publication:
Granted Patents in US and Europe

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