

CALSIMU_{TECH}



Introduction

The Calculation and Simulation Technology group (CalSimu-Tech) is a start-up that is focused on applying Computational Material Science tools in a professional and optimal way. Our goal is to design and/or help to design high quality functional materials at nanoscales. Our strategy maps the relationship between materials structures and their physico-chemical properties obtained from quantum mechanical calculations, all benefitting from our prior years of experience in multiple fields.

Over the past three decades, nano-materials-based devices have enabled society-changing technological advances. To keep up with the ever-increasing demand for energy, an enormous worldwide research effort has been geared towards the discovery of new, safe, and reliable materials with greater energy densities and higher performance. However, the development of new functional materials and their debugging, in particular, have in large remained as a laborious and painfully slow process. Practically it can take years if not decades for a successful material to move from its initiation, to laboratory test, to inside a commercial product, and become part of the market.

Our group integrates all the aspects of materials research from developing fundamental understandings to the design and simulating of new materials. We combine computational approaches in quantum mechanics, solid state physics, thermodynamics and statistical mechanics into a unified research strategy to investigate materials in the multiple fields dealing with nano-structures, including fuel cells, batteries, catalysts, and solar cells. We are the only group with years of industrial level expertise in high-throughput screening of battery materials in Iran, and among a few in the world. Our efforts within the CalSimu-Tech Research Group accelerates this process through replacing isolated insights with a systematic approach for the prediction, characterization, and debugging of known or novel materials. The CalSimu-Tech Research Group mission contributes to the nanomaterials quest by developing robust computational approaches to predict a wide range of properties such as but not limited to voltage profiles, thermal stabilities, electronic and ionic conductivities, and ionic intercalation, catalytic activities, and surface adsorption strengths.

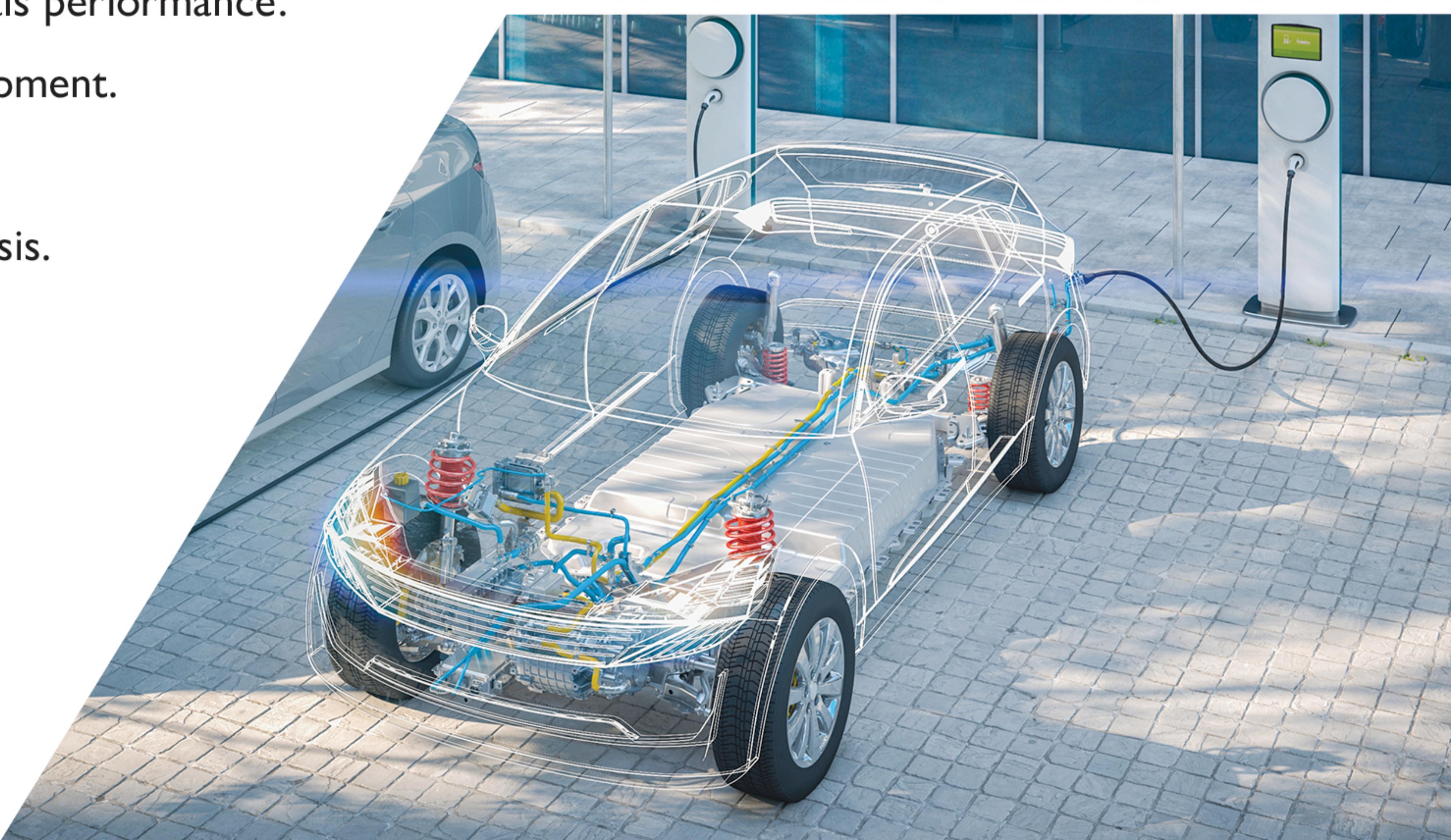
Our Main Expertise

Make quantitative insights about materials challenges based on accurate quantum computations.



Our Technical Service Methodologies, Capabilities and Skills

1. Development of materials screening criteria.
2. In-depth analysis of bottlenecks in materials performance.
3. Molecular dynamics and force field development.
4. Ab-initio thermodynamics.
5. Ab-initio spectral benchmarking and analysis.
6. High-throughput screening of materials.





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Our Technical Service Procedure

- 1 Break device into known materials structures.
- 2 Model atomic structure of all materials.
- 3 Pre-process to create input files for computations.
- 4 Run computations to solve quantum mechanical equations.
- 5 Post-process to extract raw data from output files.
- 6 Analyze and propose materials properties.

Our Consultation Service Features

1. we translate a material problem into a physical quantity to be calculated ourselves.
2. we design quantum computations that directly evaluate the target quantity ourselves.
3. we perform quantum computations in a systematically and reliable manner.
4. we post-process and interpret the numerical results professionally.
5. we convey the so-found solutions our clients.
6. we do all the above within our own group, and can do them in a wide range of fields.

Need additional information?

Feel free to contact us should you have questions or

require further information on specific topics.

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