Computational Materials Science

Activities related to Computational Materials Science span over **many length-scales** (from Ångströms to meters) and employ methods from **quantum mechanics**, over **molecular** and **mesoscale modelling** to continuum methods such as **computational micro-mechanics and fracture mechanics**. We use **machine-learning (ML)** and **data-driven** approaches employing **high-performance supercomputers** located around the globe.


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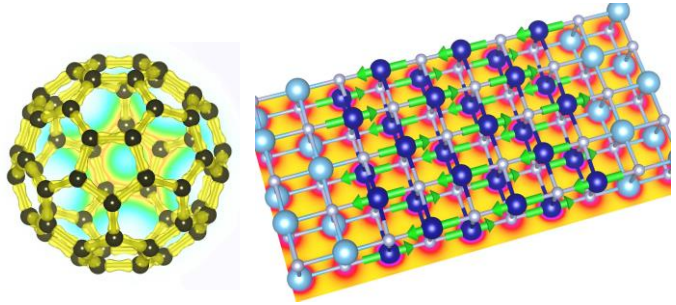
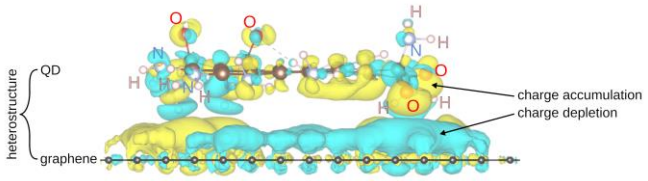
Electronic structure and bonding

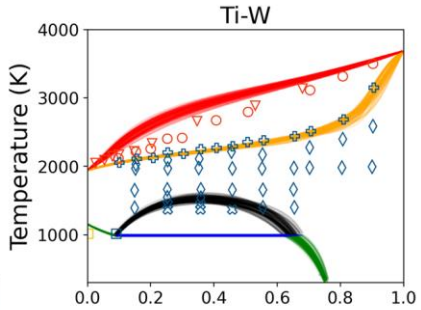


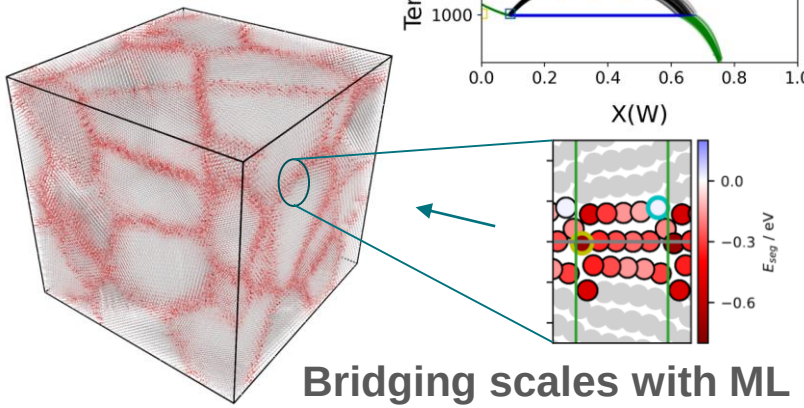
Electronic and atomistic structures



Microstructural design and ML

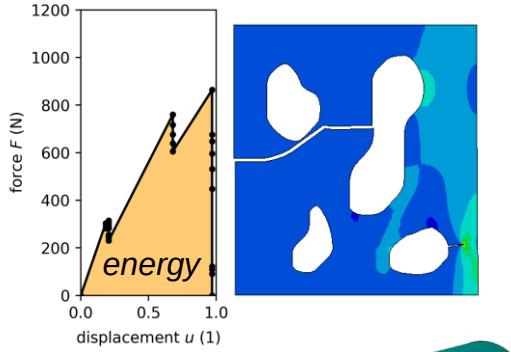
Inferring phase diagrams





Bridging scales with ML

Fracture mechanics



Re-initiating cracks

Interlocking bricks

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