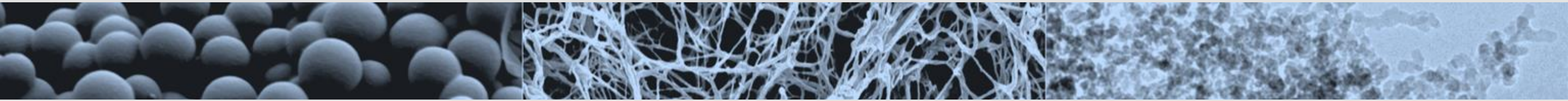


# Nanostructure under pressure: Molecular Insights into the Mechanical Behavior of Aerogel Cathodes

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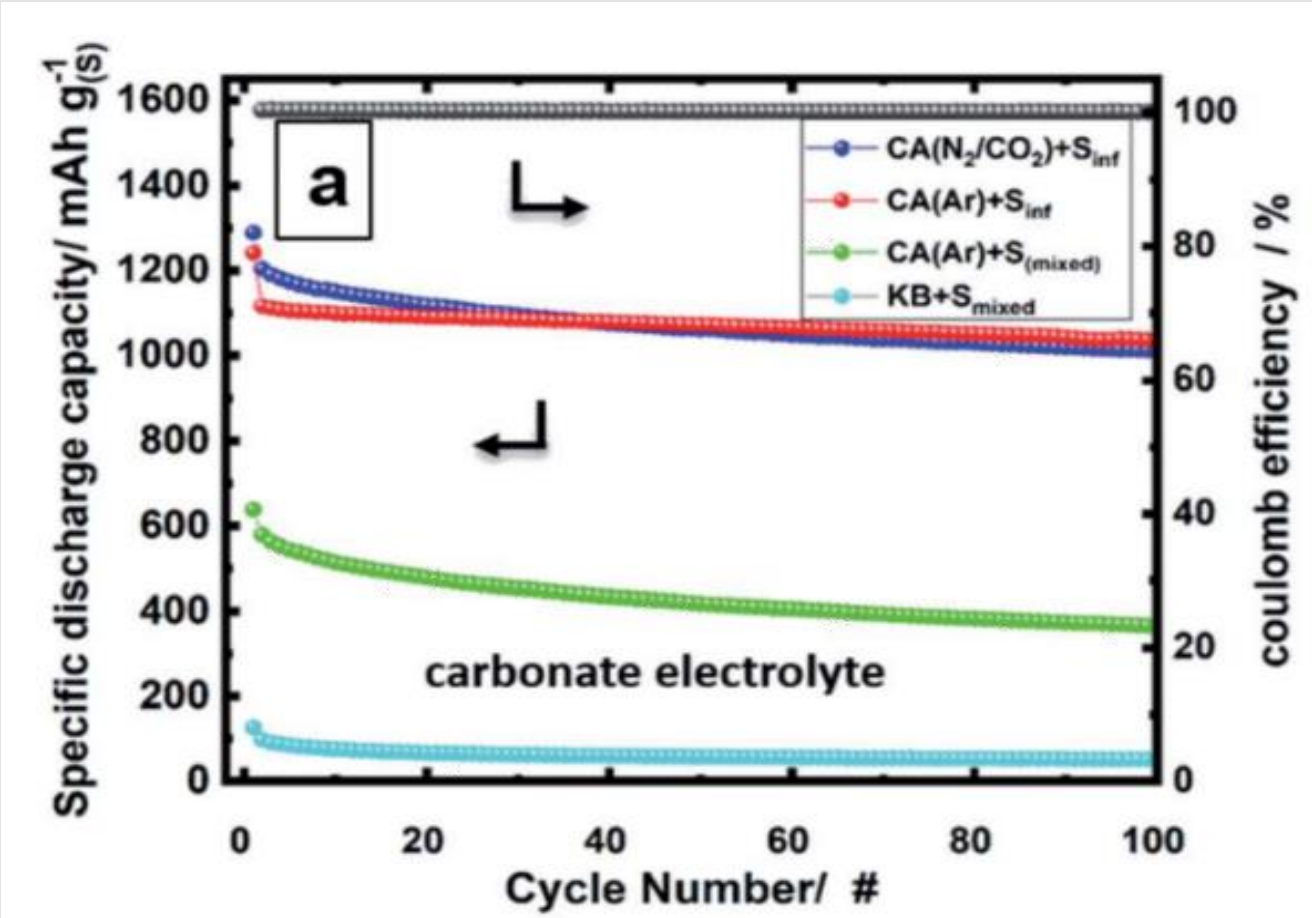
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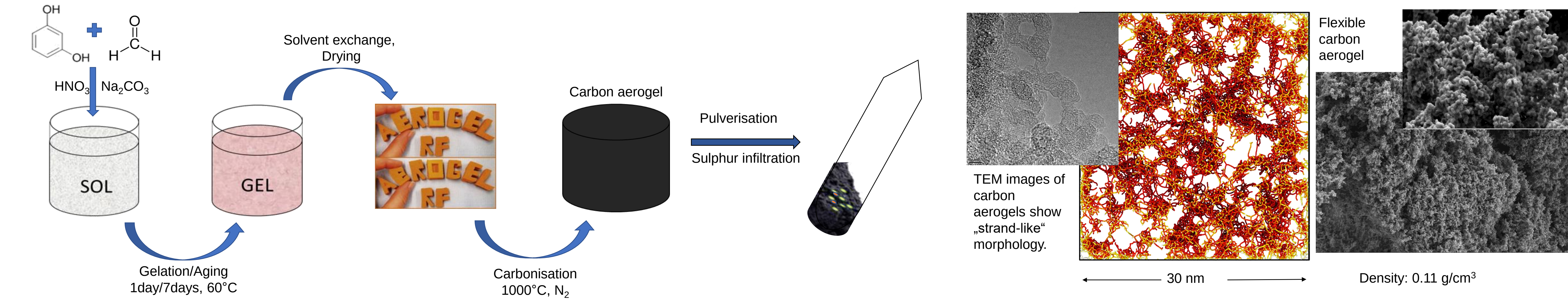
## Use of computational methods to design porous carbon nanostructures resembling carbon aerogels and study their mechanical properties for potential applications in batteries

- Carbon aerogels (~ 99.9% porosity) exhibit a large surface area, a high pore volume and high electrical conductivity. These properties make them an excellent candidate for a cathode material for Metal-Sulphur batteries.
- Sulphur as active material in the positive electrode achieves theoretical gravimetric energy density and capacity of 2600 Wh kg<sup>-1</sup> and 1675 Ah kg<sup>-1</sup> by conversion reaction and formation of polysulfides.
- In metal-sulphur batteries, the conversion reaction of sulphur and the formation of M<sub>x</sub>S cause a large volume expansion of about 80%, in nanopores (~1-5 nm), resulting in possible failure of the porous carbon network. Experimental techniques are limited in revealing the mechanical behavior of aerogels at particle level.
- Computational studies of nonlinear and inelastic mechanical behavior these nanostructured materials at molecular level provide insights into the unique structural properties and applications towards their optimization.

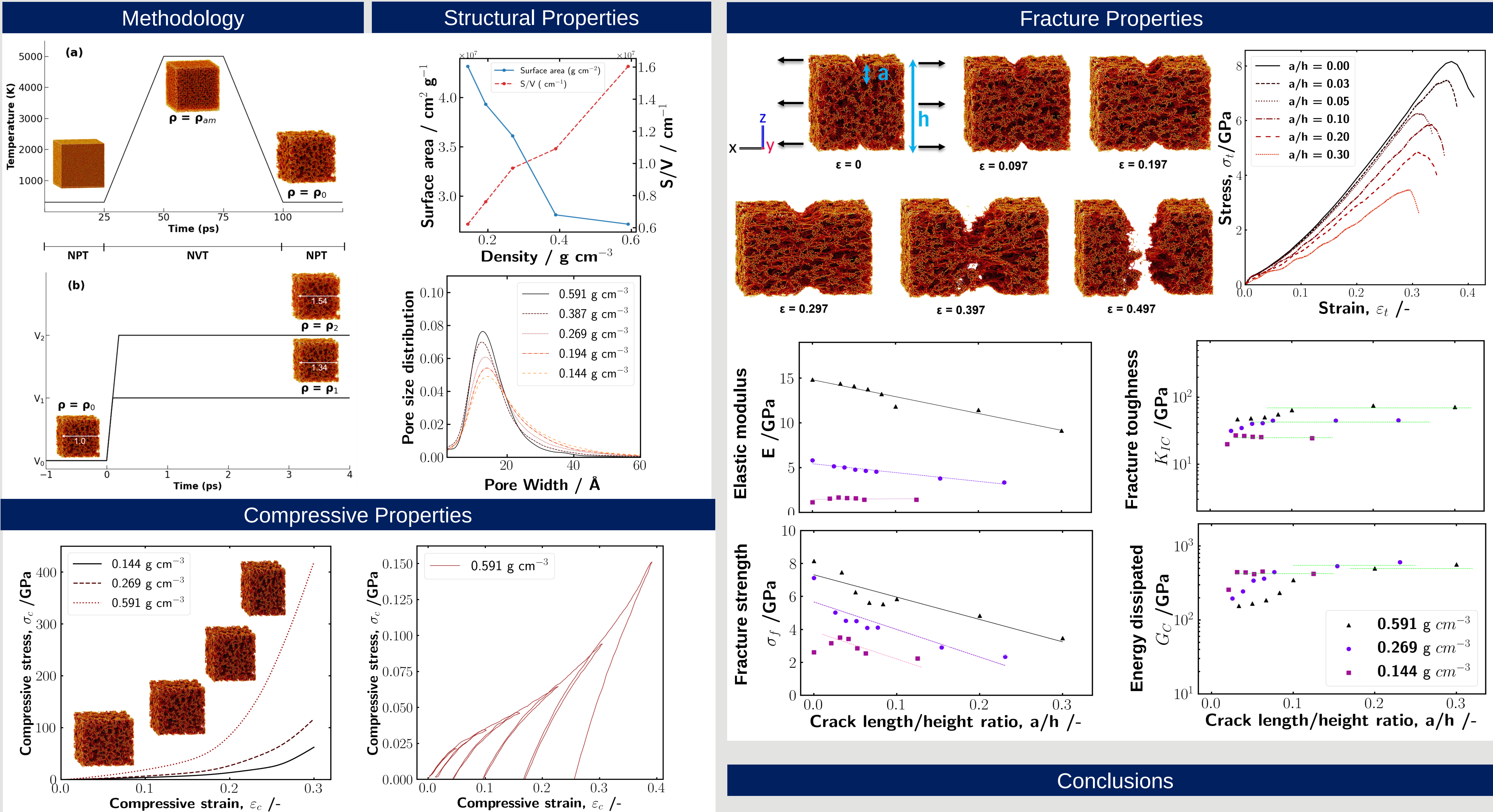


Discharge capacity and Coulombic efficiency as a function of cycle number at 0.3C rate of different carbon materials [1]

## Synthesis and characterization of carbon aerogels



## Computational mechanical characterization of porous carbon nanostructures

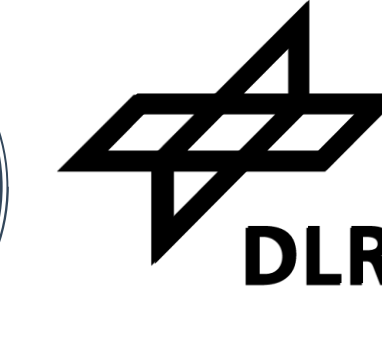


- First results on a first-of-its-kind molecular study on carbon aerogel like nanostructures with varied densities are presented which describes the molecular structural features of carbon.
- Fracture toughness and energy release rate of the models show convergence behavior beyond an a/h threshold of 0.1. These parameters are material density dependent.
- High hysteresis during cyclic compression indicate inelastic behavior of molecular nanoporous carbon.
- Stability of the simulated molecular models up to 20 % deformation indicate excellent resistance to mechanical stresses.
- This study provides crucial information about the material at a molecular level for predicting their lifespan under repeated loads when used as a cathode material.

### References

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