Self-Assembly Of Lobed Colloidal Particles Into Porous Morphologies

Brunno C. Rocha and Harish Vashisth
University of New Hampshire, Durham, New Hampshire
Email: brunno.rocha@unh.edu | harish.vashisth@unh.edu

INTRODUCTION

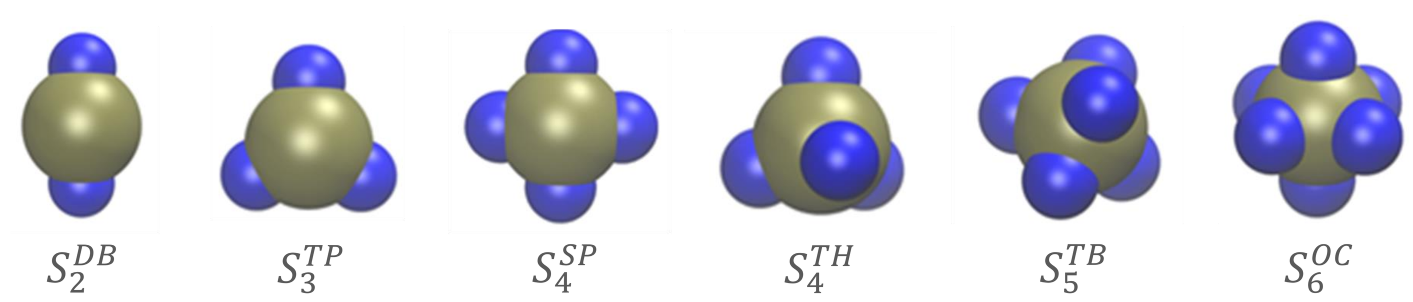
Self-assembly is a process through which particles in a system spontaneously form organized structures. A careful design of the physical characteristics of the particles can promote the formation of macrostructures with desired properties[1].

We aim to:

- Characterize the morphologies and porosities of the macrostructures obtained via self-assembly of lobed colloidal particles.
- Identify the conditions that lead to the formation of advanced materials with desired properties for practical applications.

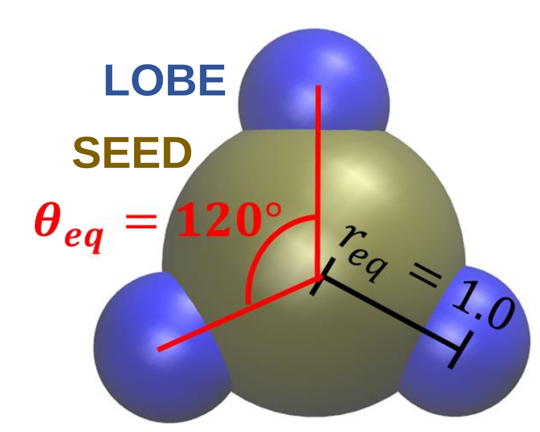
METHODS

Langevin Dynamics simulations of different lobed particles were performed under several conditions of temperature, interparticle interactions, and dispersity[2-5] using HOOMD-Blue software[6].



Seeds and lobes in the particles are modeled as individual beads, and the fixed shapes of the particles are maintained using harmonic bonds and angles:

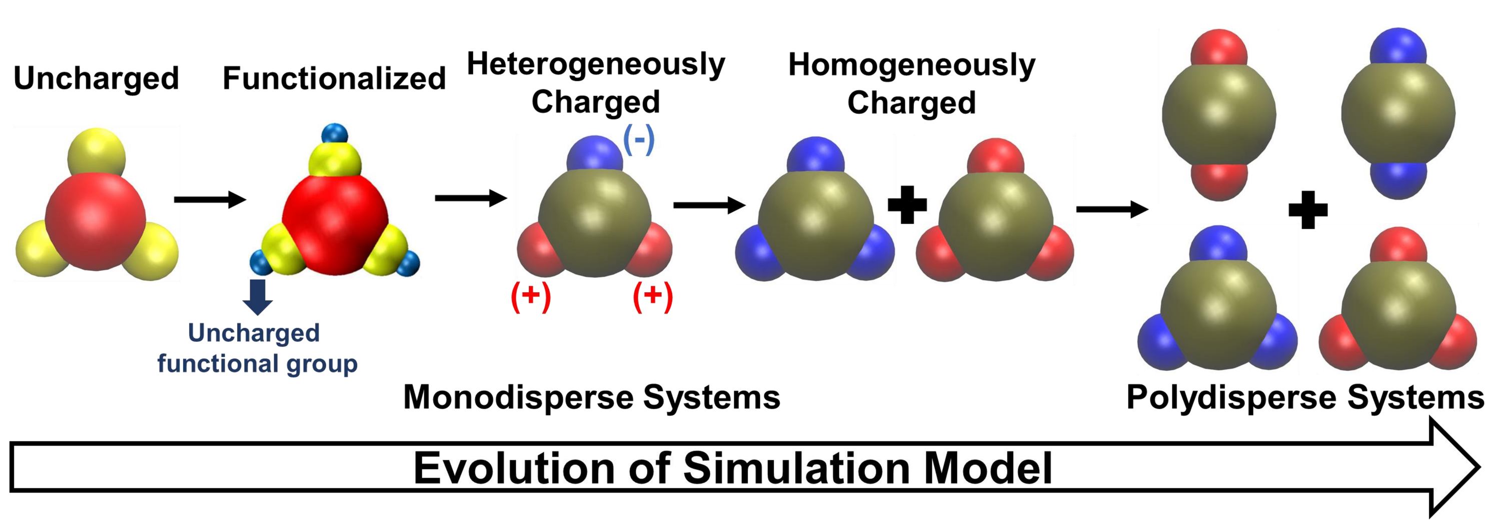
$$\sum_i k_r (r_i - r_{eq})^2 + \sum_i k_\theta (\theta_i - \theta_{eq})^2$$



The interactions between the particles are mediated by the short-ranged Surface Shifted Lennard-Jones potential and the long-ranged Coulomb potential:

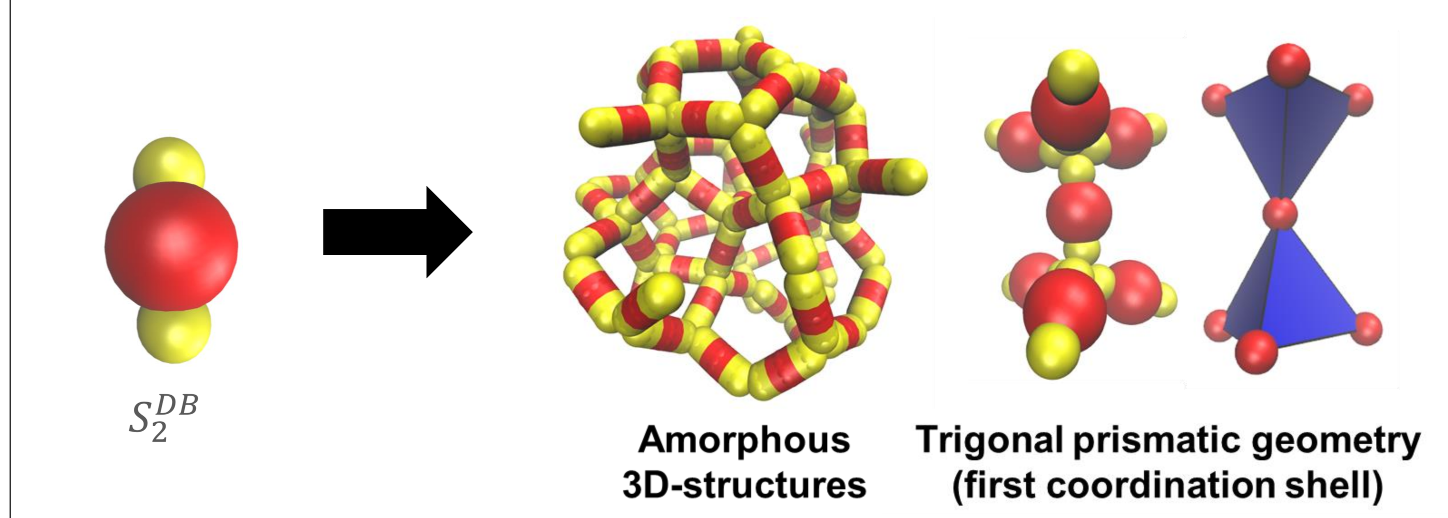
$$\sum_i \sum_{j \neq i} 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij} - \Delta} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij} - \Delta} \right)^{6} \right] + \sum_i \sum_{j \neq i} \frac{q_i \, q_j}{4\pi\epsilon_0 \epsilon_r} \frac{1}{r_{ij}}$$

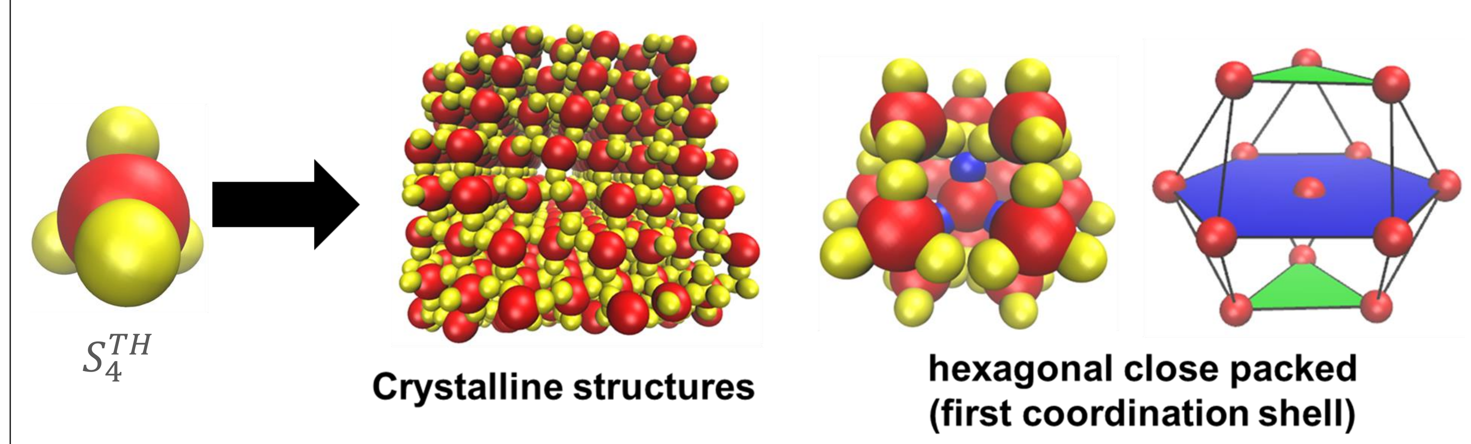
MODELS



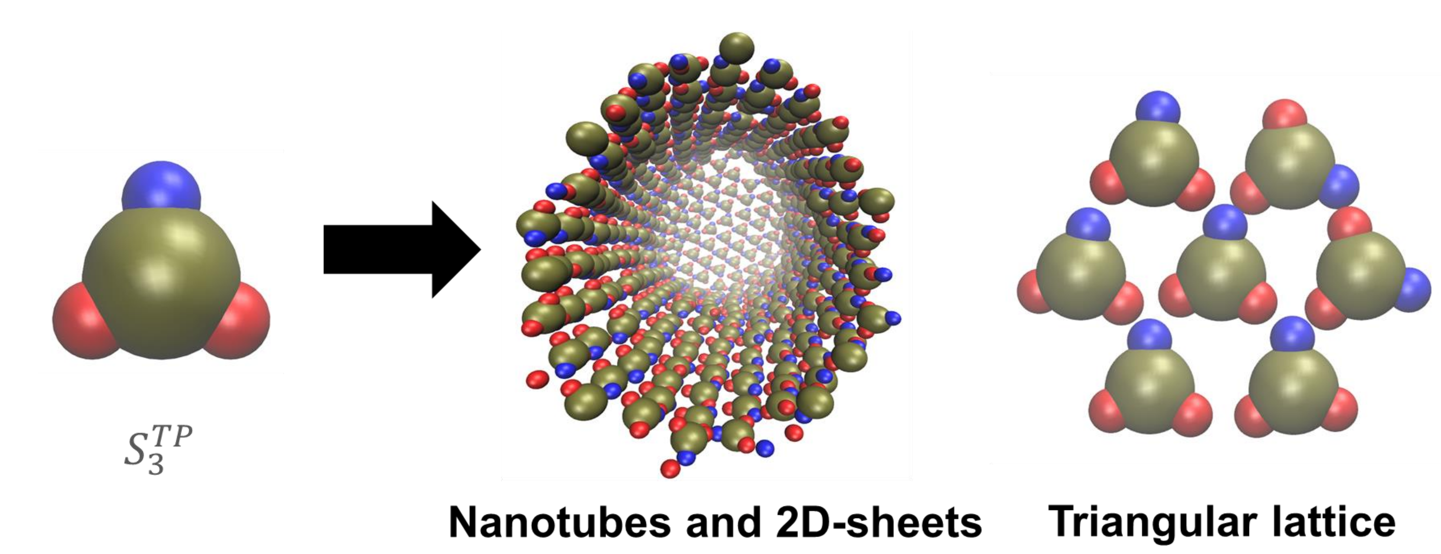
RESULTS

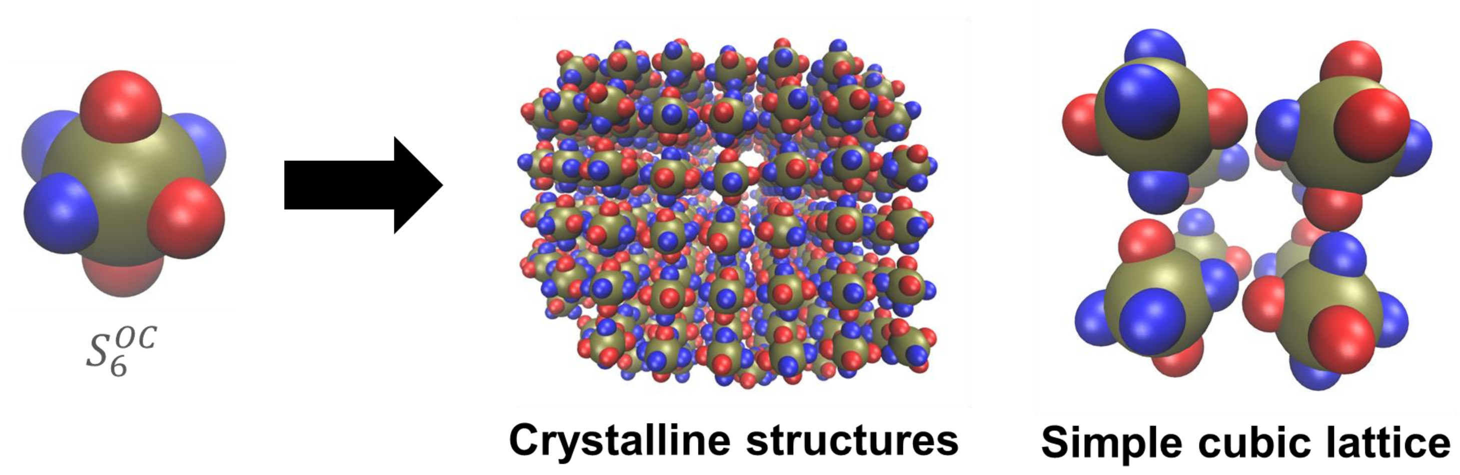
Monodisperse Systems of Uncharged Particles[2]



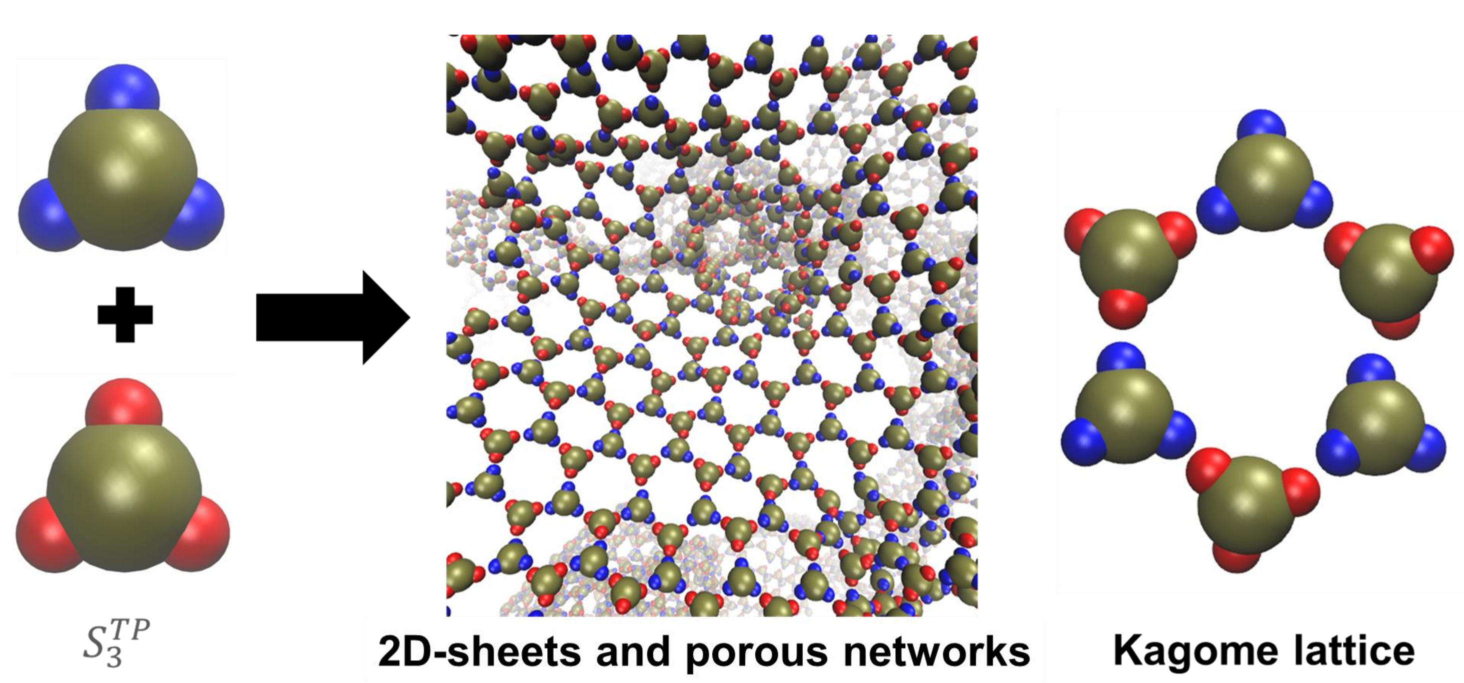


Monodisperse Systems of Heterogeneously-Charged Particles[3]

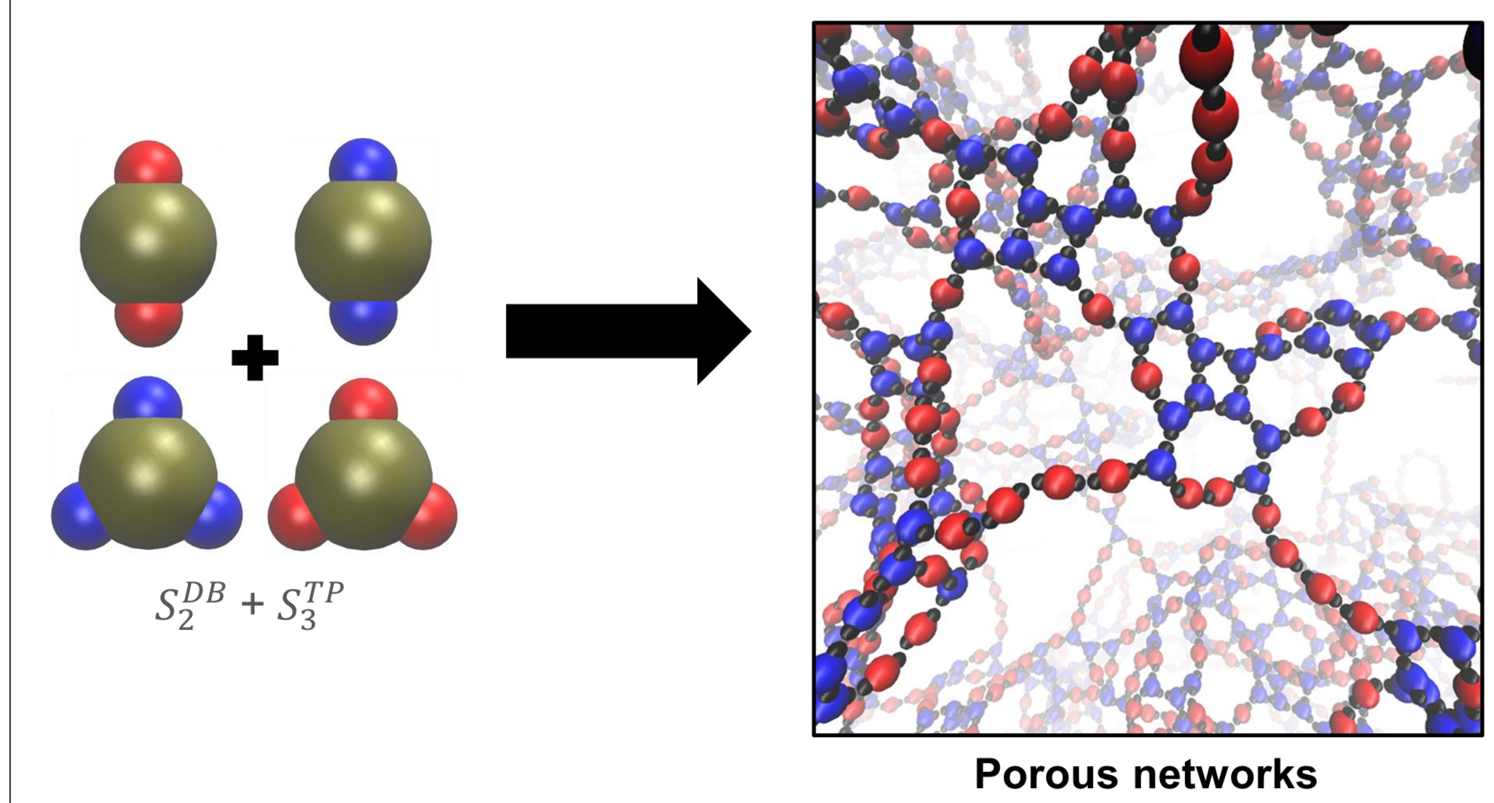




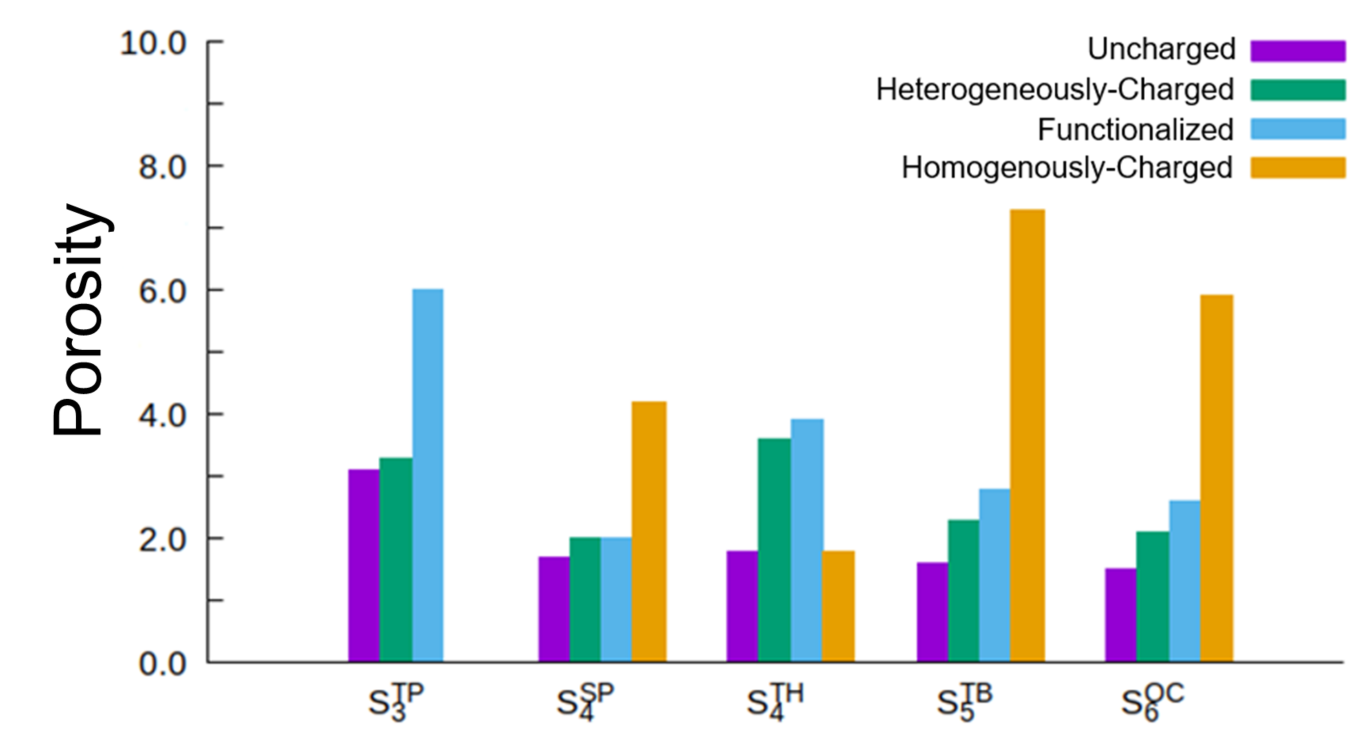
Monodisperse Systems of Homogeneously-Charged Particles[4]



Polydisperse Systems of Homogeneously-Charged Particles



Enhanced porosity with charged lobes



CONCLUSIONS

- A wide variety of morphologies and porosities can be obtained by tuning the distinct parameters of the simulations.
- Monodisperse systems of charged S_3^{TP} and polydisperse systems in general form highly porous crosslinked networks.

REFERENCES

[1] Rocha, B. C.; Paul, S.; Vashisth, H. *Entropy* **2020**, *22*, 877.
[2] Paul, S.; Vashisth, H. *Soft Matter* **2020**, *16*, 5, 1142-1147.
[3] Rocha, B. C.; Paul, S.; Vashisth, H. *J. Phys. Chem. B* **2021**, *125*, 12, 3208-3215.
[4] Srivastava, A.; Rocha, B. C.; Vashisth, H. *Front. Phys*. **2022**, *10*, 936385.
[5] Gorai, B.; Rocha, B. C., Vashisth, H. *JOM* **2021**, *73*, 2413-2422.
[6] Anderson, J. A.; Glaser, J.; Glotzer, S. C. *Comput. Mater. Sci*. **2020**, *173*, 109363.

ACKNOWLEDGEMENTS

Funding: NSF EPSCoR OIA-1757371.
Computational Resources: BioMade HPC.
Collaborators: Drs. S. Paul, A. Srivastava, and B. Gorai.