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Generating multi-modal pore size distributions for low-density micro-porous carbons using virtual void method in quenched molecular dynamics simulations

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The creation and properties of micro-porous carbons are of extreme importance for optimizing the performance of battery and supercapacitor electrodes, as well as vehicular hydrogen storage. In many cases, it is difficult to establish the microscopic structure of experimentally manufactured porous carbons. Atomistic simulation methods with reactive potentials have shown promise to fill this knowledge gap by creating realistic porous carbon structures. However, thus far such models have been unable to reproduce **low-density microporous carbon** structures due to clustering of atoms in high density regions, resulting in a small number of mesopores. Recently, we presented a new method using virtual voids, generating excluded volume by a soft repulsive potential which is progressively decoupled from the carbon atoms (Luo et al., 2021). This allows us to prevent densification and to create disordered carbon models with porosities up to 90%. We vary the size and density of the virtual voids and show that the mean of the pore size distribution and the accessible surface area can be controlled. By choosing the desired porosity and virtual void size, we created amorphous carbon models with mean pore sizes ranging from 10 to 32 Å, which agree favourably with experimental pore sizes for low-density microporous carbons. Our key findings were as follows: 1. Using the traditional quenched molecular dynamics simulation method, we confirm that carbon atoms are likely to accumulate in high density regions, preventing the formation of microporous structures [Ranganathan et al.,2017]. When using virtual voids, the carbon atoms and pores can be distributed uniformly over the whole system to generate microporous carbon with an approximately Gaussian pore size distribution and porosity up to 90%. The addition of virtual voids produced no significant effects on the short-range bonding structure characteristics; 2. Using different sized virtual voids, we gain control over the pore size distribution and surface area of the final structure. A Gaussian function was fit to the pore size distributions, which worked particularly well for smaller virtual void radius. Almost entirely microporous structures, with pore sizes < 20 Å, could be obtained using a virtual void radius of 3-4 Å. At a density of 1 g/cc, mean pore sizes ranging from 10.3 Å to 21.6 Å were found using virtual void radii from 3 Å to 10 Å, respectively. Here we extend our recent work and generate **multi-modal pore size distributions** for low-density porous carbons, using multi-modal distributions of virtual voids. This allows us to make more accurate comparisons with experimentally generated micro-porous carbons, which often have a wide distribution of pore sizes. Indeed, by using a combination of up to three different virtual void diameters, see Fig.1, we are able to create amorphous porous carbon structures with pore size distributions closely resembling experimental results. This enables us to create a comprehensive library of porous carbon structures using our multi-modal virtual void method, complementing the limited number of experimentally generated porous carbons. In turn, this may allow us to design **optimal carbon electrode structures** with respect to electrolyte permeability and carbon surface area.

Participation

In-Person

References

Luo, Z., Burrows, S.A., Fan, X., Smoukov, S.K. and Boek, E.S., 2021. Virtual voids method to generate low-density microporous carbon structures using quenched molecular dynamics simulation. Carbon, 183, pp.438-448.

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