Modern 2D anode materials for efficient energy storage systems

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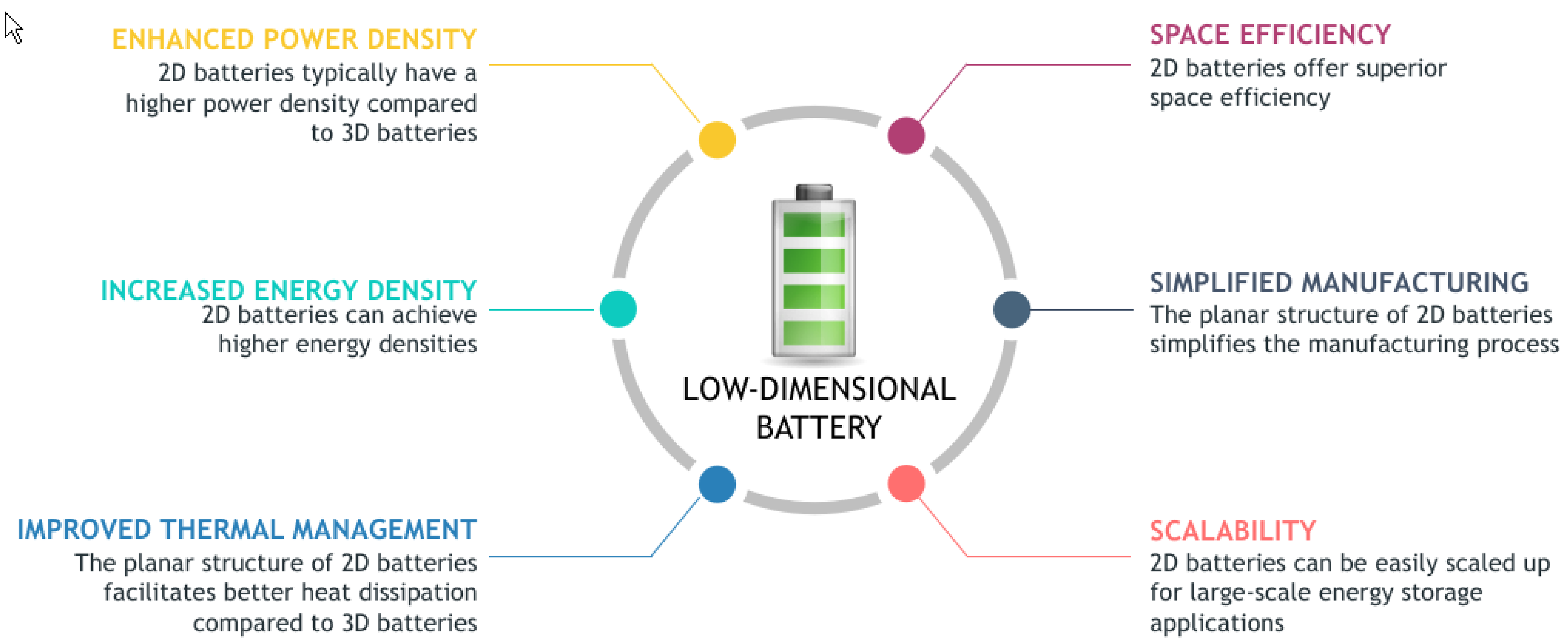
Advantages of low-dimensional batteries

Low-dimensional batteries, such as two-dimensional (2D) structures, offer several advantages over traditional three-dimensional (3D) battery architectures.

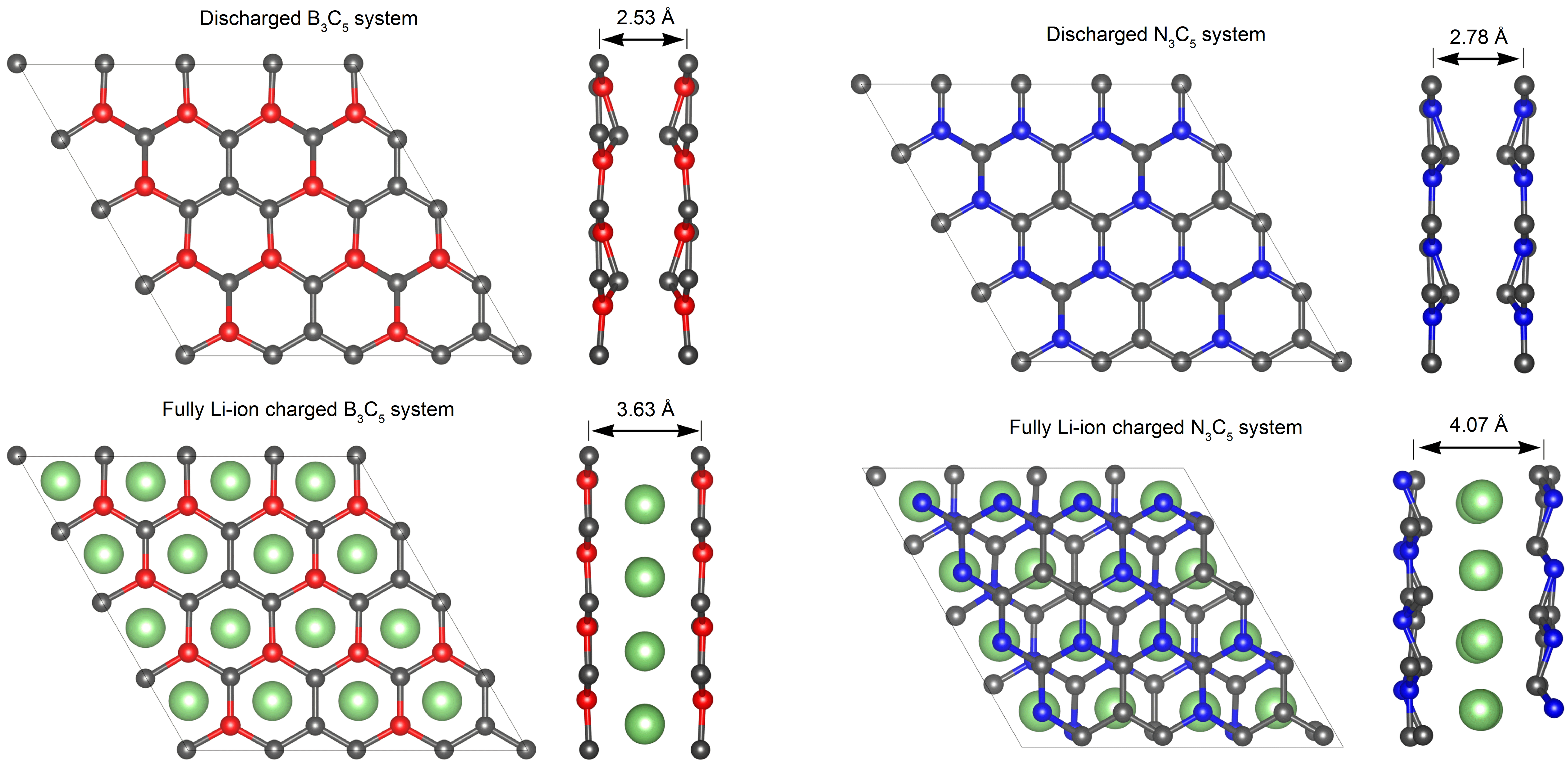


Methods

- Particle Swarm Optimization
- Density Functional Fheory
- Density-Functional Perturbation Theory
- Ab-initio Molecular Dynamics

Project of ENVIRONMENTAL SIGNIFICANT

B_3C_5 and N_3C_5 systems: candidates for anode materials for lithium-ion batteries



Atomic structure (top and side views) of pristine B_3C_5 (N_3C_5) bilayer and Li-intercalated B_3C_5 (N_3C_5) bilayer.

The most important results

The maximum theoretical specific capacity (C) was computed via the following equation:

$$C = \frac{nzF}{\mathrm{M}_{\mathrm{X_3C_5}}},$$

where n is the number of intercalated Li atoms, z is the valence number, F is the Faraday constant, and $\mathrm{M}_{\mathrm{X_3C_5}}$ is the molar mass of B_3C_5 or N_3C_5 bilayer. We achieved a high theoretical capacity of **580 mAh/g** and **525 mAh/g** for B_3C_5 and N_3C_5, anodes. The obtained results are much larger compared to these of commercially used graphite (372 mAh/g) or TiO_2 (335 mAh/g).