

## Advances in heterocyclic chemistry for high-performance energy materials: A review of green synthesis and functional applications

Induja Mishra<sup>1,2\*</sup>, Pashupati Nath<sup>1,2\*</sup>, Ajay Singh<sup>1</sup>, Vinay Kumar<sup>3</sup>, Sameer Chandra<sup>4</sup>, Nilesh Pandey<sup>5</sup> and S. R. Swarna<sup>6</sup>

<sup>1</sup>Department of Chemistry, School of Applied and Life Sciences, Uttarakhand University, Dehradun, Uttarakhand, India

<sup>2</sup>UIT, Uttarakhand University, Dehradun, Uttarakhand, India

<sup>3</sup>University School of Agriculture Science Rayat Bahra University, Mohali, Punjab, India

<sup>4</sup>Department of Botany, School of Sciences, IFTM University, Moradabad, Uttar Pradesh, India

<sup>5</sup>Post Graduate College, (VBS Purvanchal University), Ghazipur, Uttar Pradesh, India

<sup>6</sup>JSS Academy of Higher Education and Research, Mysuru, Karnataka, India

**ABSTRACT** Heterocyclic materials have developed essential structural building blocks for the future generation of sustainable energy devices owing to their basic adaptability and customizable electronic architectures. The combination of heterocyclic materials with modern energy technologies, including sophisticated metal-ion (Li/Na) batteries, fuel cells, hydrogen storage systems, and perovskite solar cells, is systematically observed in this review. This paper highlights the distinctive structure-property correlations of  $\pi$ -conjugated and redox-active heterocycles, predominantly quinones, azoles, pyrroles, and porphyrins in addition to their function in enlightening thermal stability and charge carrier dynamics. Moreover, this work highlights the shift to “Green-by-Design” approaches, underlining the utilization of biocatalysis, mechanochemical paths, and deep eutectic solvents to diminish the environmental E-factor. Developing 2026 research areas, such as waste-to-energy valorization of furans derived from biomass and artificial intelligence-driven retrosynthetic optimization, are specified a lot of consideration. This assessment offers an approach for fluctuating the global energy environment toward sustainable and uncontaminated systems by assimilating heterocyclic engineering with the circular economy’s beliefs.

**KEY WORDS** Sustainable heterocyclic chemistry, Green synthesis and E-factor, Structure-property relationships, Redox-active materials,  $\pi$ -conjugated systems, Energy storage and conversion, Perovskite and organic photovoltaics, Waste-to-energy valorization, Artificial intelligence-driven reaction optimization.

**How to cite this article:** Mishra, I., Nath, P., Singh, A., Kumar, V., Chandra, S., Pandey, N. and Swarna, S.R. Advances in heterocyclic chemistry for high-performance energy materials: A review of green synthesis and functional applications. *Indian J. Heterocycl. Chem.*, 2026, 36, 171–178, <https://doi.org/10.59467/IJHC.2026.36.171>