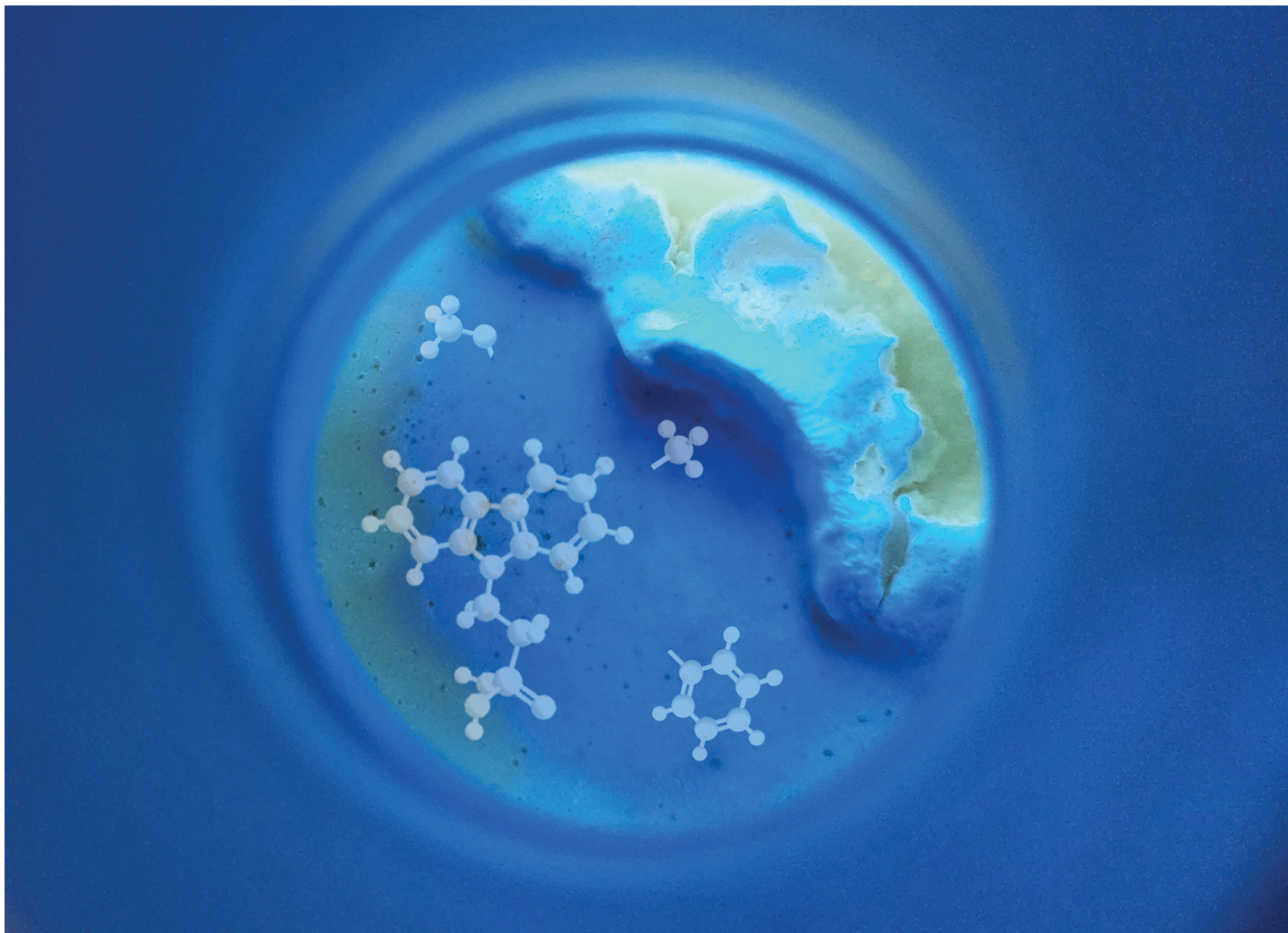




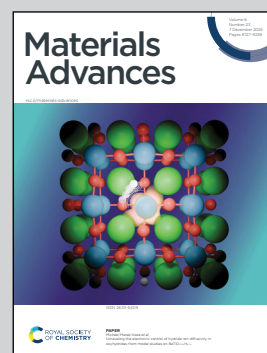
Showcasing research from Kaunas University of Technology (KTU), Lithuania in collaboration with Helmholtz-Zentrum Berlin (HZB).

Screening of the carbazole-based phosphonic acids in perovskite solar cells: impact of the substitution pattern on device performance

This work presents a comparative study of nine carbazole-based phosphonic acids used as self-assembled monolayers (SAMs) in p-i-n perovskite solar cells. By varying methyl, methoxy, and phenyl substituents at different positions, the study reveals that molecules substituted at the 3,6-positions achieve the highest fill factors and improved charge extraction, supported by trSPV and PESA analyses. A threshold ionization potential of -5.45 eV was identified, beyond which device performance declines. This work provides insightful knowledge that can contribute to further investigations and design of phosphonic acid-based materials.

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Mater. Adv., 2025, **6**, 8921.