Abstract

The recent fast development of perovskite solar cell (PSC) technology has highlighted the significance of the use of hole transport materials (HTM) in the improvement of power conversion efficiency (PCE) and the stability of the device. Traditional HTMs like Spiro-OMeTAD have good energy characteristics but the intrinsic hole mobility is low, it can be oxidized easily. This study overcomes these shortcomings by modeling new carbazole-based HTM with donor-acceptor structures. Seven new carbazole based HTMs were theorized with different substituents (methoxy, fluorine, methyl) on their side units at different positions to evaluate their optoelectronic properties and charge transport. DFT studies were used to analyze their HOMO-LUMO levels, band gaps, and molecular electrostatic potentials (MEPs) and TD-DFT was used to analyze their optoelectronic properties. The global reactivity parameters (ionization energy, dipole moment, electron affinity, hardness and softness and electrophilicity index) were also calculated to study their stability and charge transfer properties. Overall, all the molecules exhibited suitable HOMO level that to extract holes effectively. The C5 (N2,N2,N7,N7-tetrakis(4-(9H-carbazol-9-yl)phenyl)-9-methyl-9H-carbazole-2,7-diamine) molecule showed a good band gap, absorption spectra (lambda max), and high charge delocalization. C5 showed good hole selectivity while C6 molecule, its fluorine substituted derivative, showed greater recombination resistance but had reduced band gaps. This computational work is able to find some promising carbazole-based HTMs, which present cost-efficient, stable, and effective proxies in the next-generation PSCs