New thiophene-based poly(azomethine)s bearing tetraphenylsilane moieties along their backbone. Optical, electronic, thermal properties and theoretical calculations

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A new series of conjugated thiophene-based poly(azomethine)s (PAZThAs) containing tetraphenylsilane (TPS) cores and thiophene or bithiophene moieties along the backbone were obtained from silicon-containing diamines and commercial 2,5-thiophenedicarboxaldehyde and 2,2?-bithiophene-5,5?-dicarboxaldehyde through high-temperature polycondensation reactions. Solution-processable polymers were obtained in high yields (74?96%), high average molecular weight (Mw: 2,900?22,200 g/mol), with adequate polydispersity (closed to 2), and high thermal stability (T10%: 326?488 °C). The thiophene-based PAZ showed suitable absorptions and emissions in the UV?vis range with moderate Stokes shifts (46 to 65 nm). The lower band gap value was observed for PAZ2ThA2 (1.98 eV) that is closely similar to polythiophene derivates studied in polymer solar cells (PSCs). The calculated HOMO energies values are in the range of ?5.82 eV to ?5.42 eV, while the LUMO energies ranging from ?3.56 to ?3.39 eV. Compared to fully ?-conjugated

PThs, the PAZThAs tend to possess higher LUMO energies and similar HOMO energies, which is attributable to the electronic influence of the TPS-cores. This study motivates future researches on TPS building-blocks based PAZs.

Poly(azometine)s

Polythiophenes

Silicon-based polymers

Solution-processable polymers

Energy gap

Polydispersity

Polymer solar cells

Thiophene

Average molecular weight

High temperature polycondensation

High thermal stability

Poly(azometine)s

Polymer solar cell (PSCs)

Silicon-based

Solution processable

Theoretical calculations

Polymers