DOCTORAL THESIS ABSTRACT

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This doctoral dissertation focuses on the synthesis, molecular design, and thermal characterization of phase change materials (PCMs) derived from renewable and sustainable precursors, including tartaric acid, mucic acid, glycerol carbonate, lactones (D-glucono-δ-lactone, D-ribono-γ-lactone, and D-erythro-γ-lactone), fatty alcohols, and fatty amines. The global transition towards sustainable development and low-carbon technologies has driven the search for environmentally friendly alternatives to widely used commercial PCMs, which are predominantly based on fossil-derived paraffins. Depending on their melting temperature (T_m), heat storage capacity, and stability, these materials find applications in thermal energy storage from renewable energy sources, building thermoregulation, water heating, and cold chain logistics. Although the scientific literature and the product portfolios of leading technology companies are dominated by PCMs with phase transition temperatures below 70 °C, reflecting the market maturity and commercial potential of this technology, their relatively narrow operating temperature range limits their versatility. Overcoming these limitations requires precise optimization of molecular structures, enabling the rational design of materials with specifically tailored properties.

Previous approaches to modifying organic PCMs have primarily focused on investigating the effects of alkyl chain length and branching, isomerism, molecular symmetry, and the introduction of simple functional groups, such as ester, amide, and sulfone groups. Sugar alcohols reported in the literature, which contain numerous hydroxyl (-OH) groups, form extensive hydrogen-bonding networks that contribute to exceptionally high melting enthalpies (ΔH_m), reaching up to 350 J g^{-1} for galactitol. However, their practical application is limited by poor cycling stability, a tendency towards supercooling, and difficulties in crystallization. In contrast, paraffins, fatty acids, and fatty alcohols, stabilized by van der Waals interactions, exhibit excellent reversibility of phase transitions but are characterized by relatively low melting temperatures.

The primary objective of this dissertation was to develop new PCMs by modifying the molecular structures of compounds derived from renewable resources. To achieve this, a systematic strategy involving the deliberate combination of hydroxyl-rich precursors with long alkyl chain-containing fragments was applied for the first time. This approach enabled the preparation of compounds with diverse thermal properties by controlling the relative contributions and strengths of hydrogen bonding and van der Waals interactions within their molecular structures.

The research resulted in materials exhibiting a broad range of melting temperatures (57–190 °C), high melting enthalpies (up to 221 J g^{-1}), and excellent cycling stability, demonstrated over 500 consecutive heating and cooling cycles in the case of the esters. The established relationships between molecular structure and the thermal properties of the synthesized materials provide further insight into the factors governing phase transition temperatures, melting enthalpies, and cycling stability, thereby establishing a foundation for the rational design of PCMs tailored to specific future applications.