VRIJE UNIVERSITEIT BRUSSEL

The faculty of Engineering of the Vrije Universiteit Brussel invites you to attend the public defense leading to the degree of

DOCTOR OF ENGINEERING SCIENCES

of **Zhen Liu**

The public defense will take place on **Friday 27th January 2023 at 4:00pm** in room **D.0.05** (Building **D**, Brussels Humanities, Sciences & Engineering Campus)

To join the digital defense, please click here
Meeting ID: 348 967 775 05
Passcode: 9fFnJV

PHASE BEHAVIOR AND STATE DIAGRAMS OF CONJUGATED SYSTEMS FOR ORGANIC OPTOELECTRONICS
IMPORTANCE OF INTERCALATION AND HOMOCOUPLING

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Abstract of the PhD research

Organic optoelectronics such as organic photovoltaics and organic photodetectors have seen a strong increase in both scientific studies and technological development during the past decades. However, systematic studies of the phase behavior of donor:acceptor mixtures, which constitute the active layer of these devices, and directly influences the performance, remain largely absent. This thesis focuses on the study of the complex phase behavior of such active layers, and the construction of their state diagrams, to reveal the composition-temperature-phase behavior relationships of these mixtures.

First, three defect-free donor materials, PBTTT and two novel derivatives, as well as their mixtures with PC61BM acceptor, were studied by rapid heatcool calorimetry and temperature resolved synchrotron X-Ray diffraction. This combination enables the investigation of both phase transitions and structural evolution as a function of temperature. For each mixture a the formation of a unique compound as well as eutectic behavior was observed. Taking into account this complex phase behavior, state diagrams for these three systems were constructed in a systematic way. A second part of this doctoral thesis was focused on the effect of homocoupling, common defects which originate from the synthesis procedure of push-pull low bandgap donor materials, on the phase behavior, state diagrams, and resulting device performance.

Rapid heat-cool calorimetry complemented with temperature resolved synchrotron X-Ray diffraction is proven to be a successful method to construct accurate and reliable state diagrams. Although this is a fundamental study, the developed state diagrams could be applied to thoroughly understand of donor: acceptor mixtures, and to optimize the morphology of active layers in actual devices.