Investigations on thermophysical and electronic properties of Pt-porphyrin molecular solids

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Pt-porphyrin is a class of molecules that is proposed for broad applications. For example, the most representative molecule PtOEP **(Fig. 1a**) has been used in organic electroluminescence devices [1,2], oxygen sensors [3,4], and photon upconverters [5,6]. While the structural, electronic, and electrochemical properties of PtOEP and its derivatives (e.g., **Fig. 1b** and **1c**) were reported so far [7,8], their thermophysical properties have not well been investigated. Such properties are desired to be clarified because in certain circumstances thermal deposition techniques are preferred rather than solution-based processes to make the layers or films. To elucidate their thermophysical properties, we carried out investigations on the group of molecules shown in **Fig. 1** by means of a thermo-gravimetric analysis, differential scanning calorimetry, and temperature dependent X-ray diffraction. We also studied and discussed their electronic properties including their energy levels and electron distributions (**Fig. 2**) by quantum chemical simulations. The details of our findings will be presented at the poster.

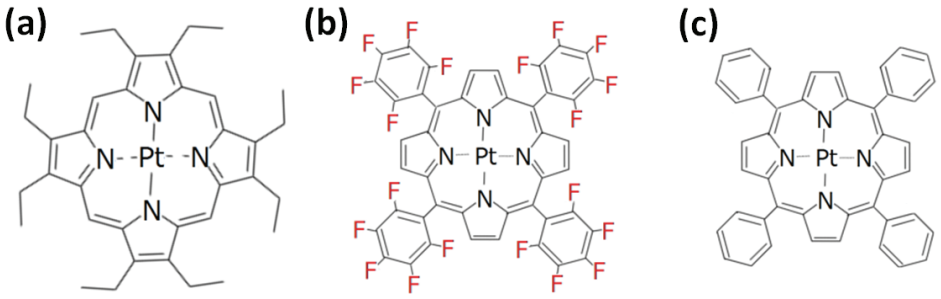

Fig. 1: Molecular structures of Pt porphyrins investigated, (a) PtOEP, (b) PtTFPP, and (c) PtTPP.

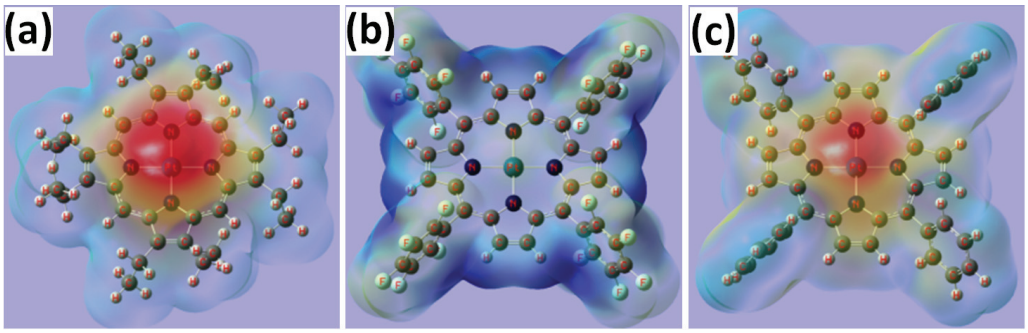

Fig. 2: Electron density distributions in (a) PtOEP, (b) PtTFPP, and (c) PtTPP calculated by Gaussian09. Here, red and blue colors represent electron rich and deficient, respectively.

[1] M. Sagal et al., *Nature Mater.* **6**, 374 (2007). [2] M. A. Baldo et al., *Nature* **395**, 151 (1998). [3] I. Okura et al., *Analyst* **122**, 81 (1997). [4] B. H. Han et al., *Anal. Chem.* **77**, 8075 (2005). [5] J. Zhou et al., *Chem. Rev*. **115**, 395 (2015). [6] T. F. Schulze et al., *Energy Environ. Sci*. **8**, 103 (2015). [7] S. W. Lai et al., *Inorg. Chem.* **43**, 3724 (2004). [8] S. K. Lee et al., *Anal. Chem*. **34**, 185 (1997).