Charge-Carrier Transport Properties in Dehydrobenzoannulene-Based 2D Conductive Metal–Organic Frameworks

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Conductive 2D metal–organic frameworks (2D c-MOFs) are layered, sheet-like coordination polymers renowned for their crystallinity, porosity, and electrical conductivity. These properties make them promising for various applications such as sensing.[1] Currently, we are exploring the construction and functional development of 2D c-MOFs comprising dehydrobenzoannulenes (DBAs) as ligands, and previously reported two novel DBA-based 2D c-MOFs, Ni-HA12 and Ni-HA18 (Fig. 1a, c).[2] These MOFs achieve BET surface areas of up to 1720 $m^2\ g^{-1}$, surpassing the previously reported maximum.

In this work, we investigated the charge-carrier transport properties of these DBA-MOFs. Band diagrams from DFT calculations revealed that the band dispersions along the intraplane direction were comparable to those of conventional sp^2-carbon-based 2D c-MOFs, suggesting that the DBA-MOFs may exhibit excellent charge-carrier transport capabilities (Fig. 1b, d). This presentation will discuss the charge-carrier transport characteristics of these MOFs, estimated from the band calculations and time-resolved terahertz spectroscopy.

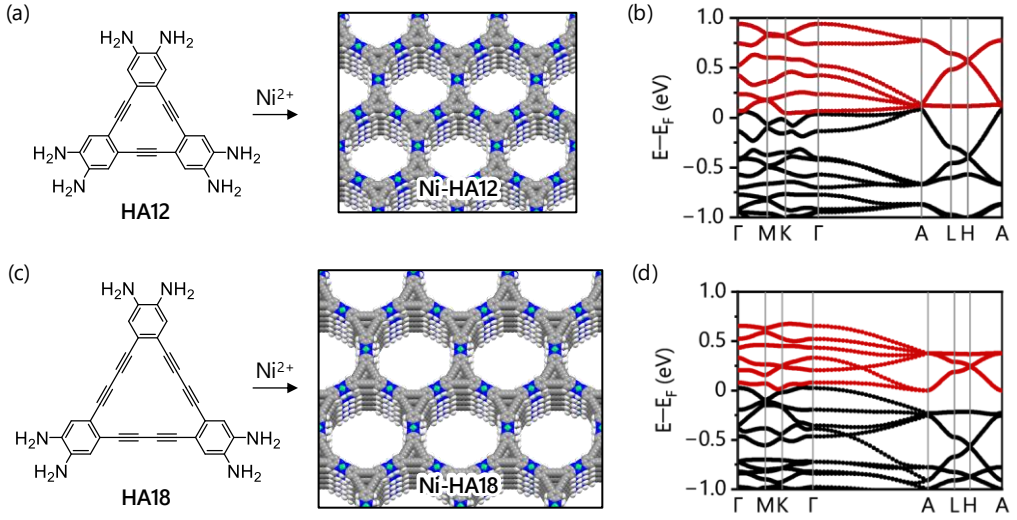

Fig. 1 Expected structures and calculated band diagrams of Ni-HA12 (a, b) and Ni-HA18 (c, d). Black and red lines in b and d indicate the valence and conduction bands, respectively.

(1) Liu, W. et al. *Chem. Eur. J.* **2024**, *30*, e202402747. (2) Ohkubo, E. et al. The 104th CSJ Annual Meeting, F1233-1pm (**2024**).