

The effect of the aliphatic carboxylate linkers on the electronic structures, chemical bonding and optical properties of the uranium-based metal organic frameworks

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Supplementary materials

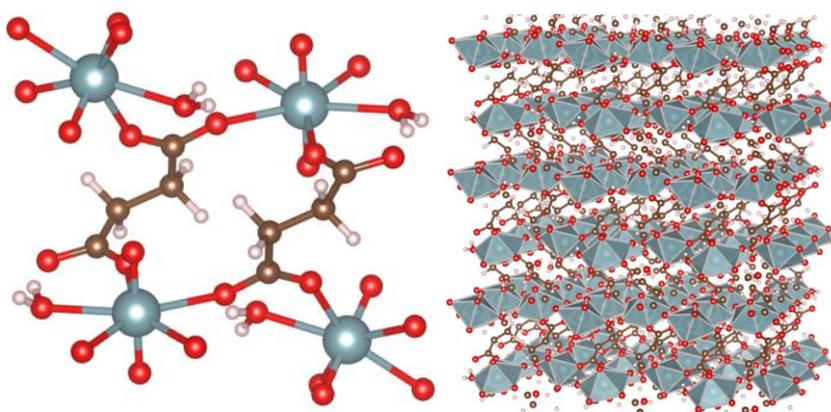


Figure S 1: The coordination environment of the uranyl inorganic building units and its connectivity to the organic linkers succinate acid (C₄H₆O₄) in MOF1 (left). The color code is as follows: Neptune for U, korma for C, red for O, and light pink for H. Polyhedral representation of MOF1 (right). Neptune pentagonal bipyramids of uranyl units are connected through succinate acid.

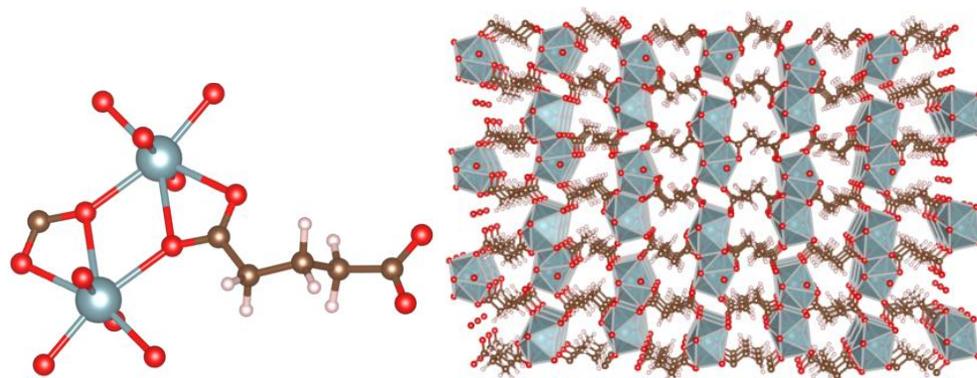


Figure S 2: The coordination environment of the uranyl inorganic building units and its connectivity to the organic linkers glutarate acid (C₅H₈O₄) in MOF2 (left). The color code is as follows: Neptune for U, korma for C, red for O, and light pink for H. Polyhedral representation of MOF2 (right). Neptune pentagonal bipyramids of uranyl units are connected through glutarate acid.

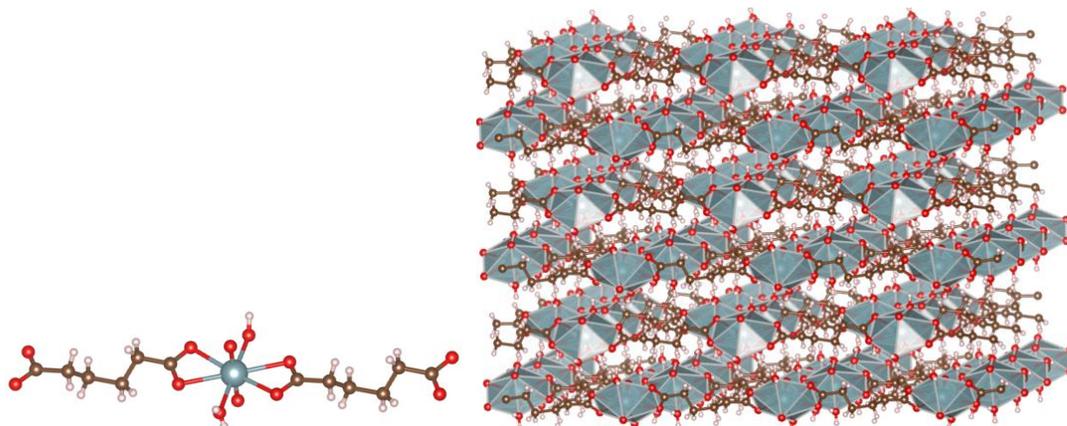


Figure S 3: The coordination environment of the uranyl inorganic building units and its connectivity to the organic linkers adipate acid ($C_6H_{10}O_4$) in MOF3 (left). The color code is as follows: Neptune for U, korma for C, red for O, and light pink for H. Polyhedral representation of MOF3 (right). Neptune hexagonal bipyramids of uranyl units are connected through adipate acid.

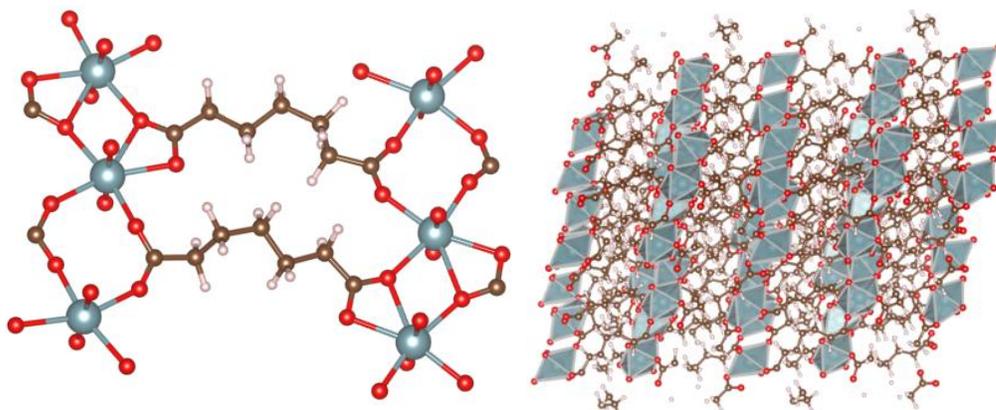


Figure S 4: The coordination environment of the uranyl inorganic building units and its connectivity to the organic linkers pimelic acid ($C_7H_{12}O_4$) in MOF4 (left). The color code is as follows: Neptune for U, korma for C, red for O, and light pink for H. Polyhedral representation of MOF4 (right). Neptune pentagonal bipyramids of uranyl units are connected through pimelic acid.

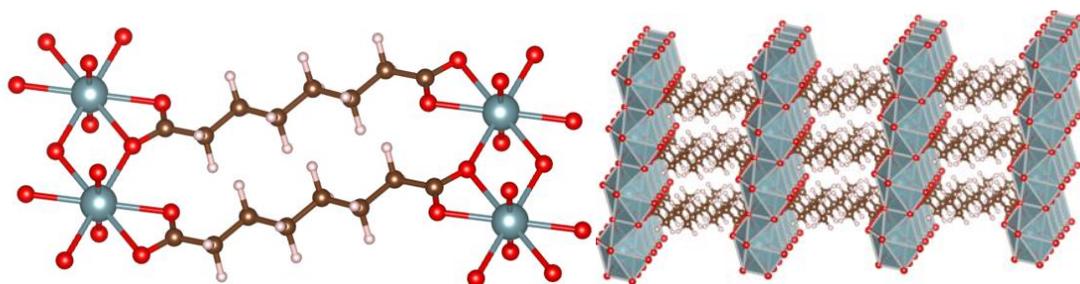


Figure S 5: The coordination environment of the uranyl inorganic building units and its connectivity to the organic linkers suberic acid ($C_8H_{14}O_4$) in MOF5 (left). The color code is as follows: Neptune for U, korma for C, red for O, and light pink for H. Polyhedral representation of MOF5 (right). Neptune hexagonal bipyramids of uranyl units are connected through suberic acid.

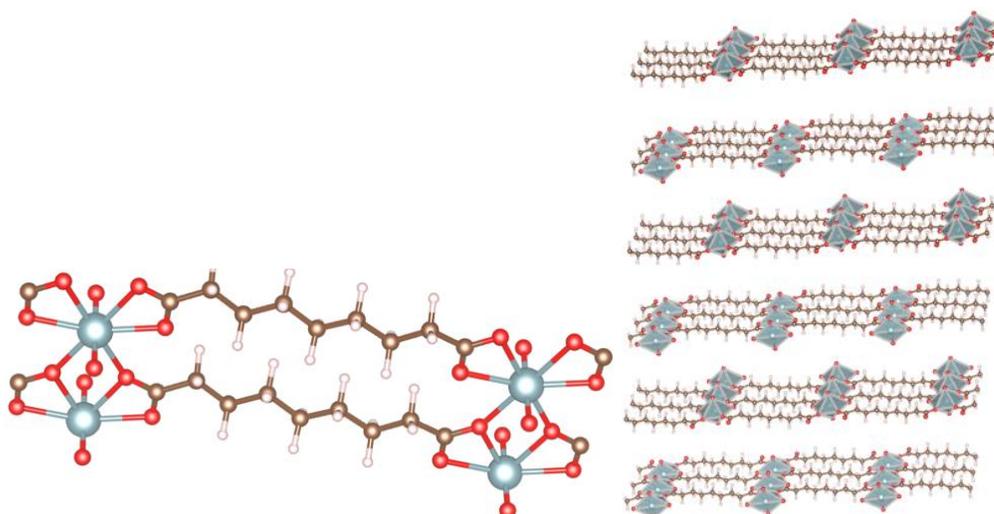


Figure S 6: The coordination environment of the uranyl inorganic building units and its connectivity to the organic linkers azelaic acid ($C_9H_{16}O_4$) in MOF6 (left). The color code is as follows: Neptune for U, korma for C, red for O, and light pink for H. Polyhedral representation of MOF6 (right). Neptune hexagonal bipyramids of uranyl units are connected through azelaic acid.

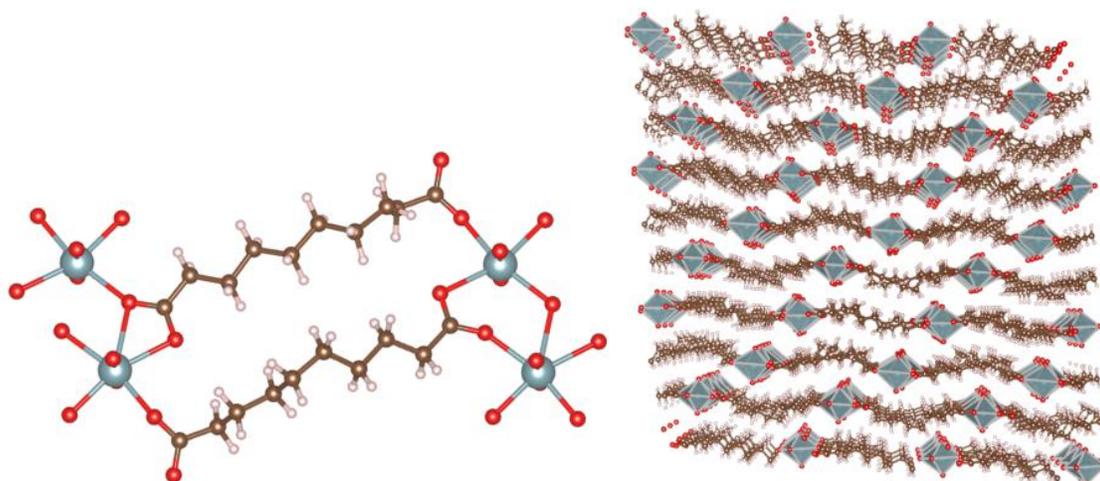


Figure S 7: The coordination environment of the uranyl inorganic building units and its connectivity to the organic linkers sebaic acid ($C_{10}H_{18}O_4$) in MOF7 (left). The color code is as follows: Neptune for U, korma for C, red for O, and light pink for H. Polyhedral representation of MOF7 (right). Neptune pentagonal bipyramids of uranyl units are connected through sebaic acid.