Metal-Organic frameworks (MOFs) are crystalline porous materials. Coordination bonds between transition metal cations and organic ligands. Applications in gas separation, sensing devices, and drug delivery.

**Experimental**
- Copper benzene-1,3,5-tricarboxylate (CuBTC) MOF was synthesized using manual LbL method at room temperature.
- Gold (Au 200nm) substrate was immersed in a solution of 16-Mercaptoundecanoic acid (16-MIDA) and ethanol for 1 hour to generate the self-assembled monolayer (SAM) with –COOH functionality.
- Layer-by-Layer method:
  - Immersion in copper acetate solution
  - Immersion in trimesic acid solution
  - Rinsing (ethanol) and drying (N₂) steps between each immersion
  - The cycle was repeated 40 times at ambient temperature

**Molecular modelling**
- Grand Canonical Monte Carlo used to obtain adsorption isotherms
- Allows comparison with experimental data

**Results**
- GCMC simulations
  - No partial atomic charges used
  - Various partial atomic charges used for comparison
  - Different isotherm shape for different charge sets
  - CHELPG® partial atomic charges used
  - Type III isotherm

**Conclusions**
- CuBTC was synthesized using manual LbL method
- GCMC simulations indicate that partial atomic charges obtained by different methods have varying effects on different MOFs

**Future work**
- The experimental method will be adjusted in order to investigate the effect of factors including temperature, concentration, immersion time etc. on crystal formation and properties
- In order to establish a systematic procedure to evaluate the effect of atomic partial charges on adsorption isotherms, GCMC simulations of CuBTC and water with different sets of partial charges

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