# DFT calculations on Cu-based metal-organic hybrid materials

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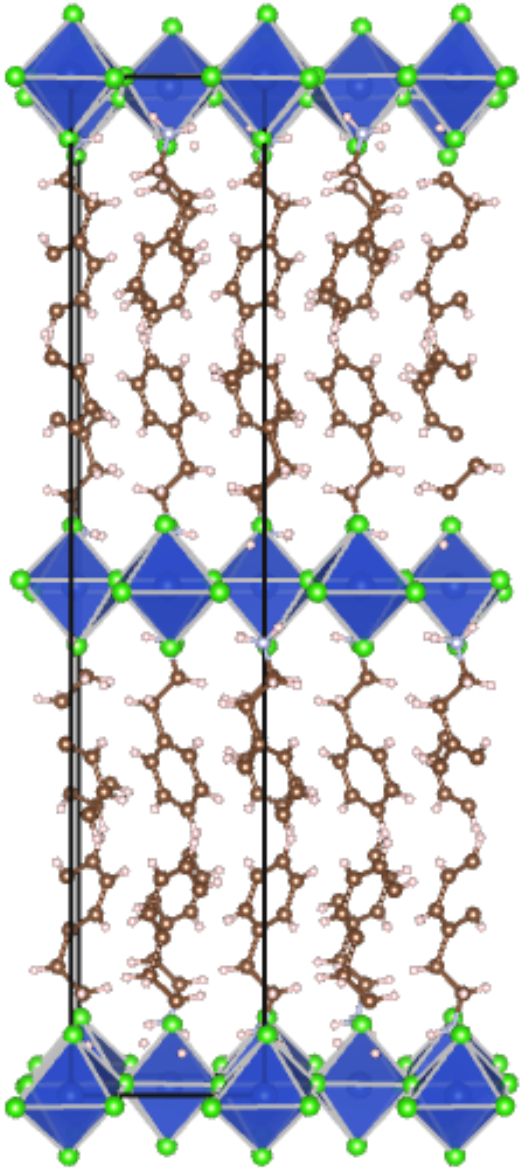
# Crystal Structure of Cu-Hybrid-*PEA*

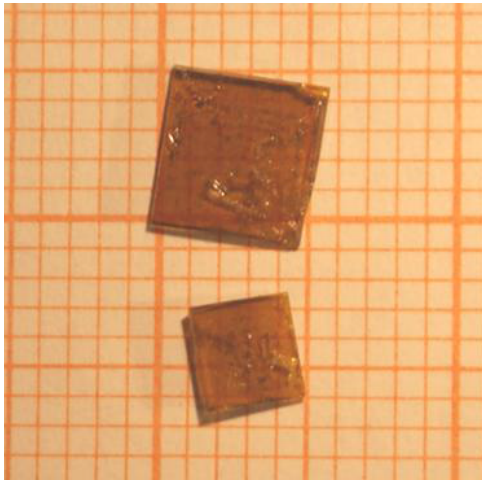


Bis-(2-Phenyl Ethyl Ammonium) tetrachlorocuprate (II)

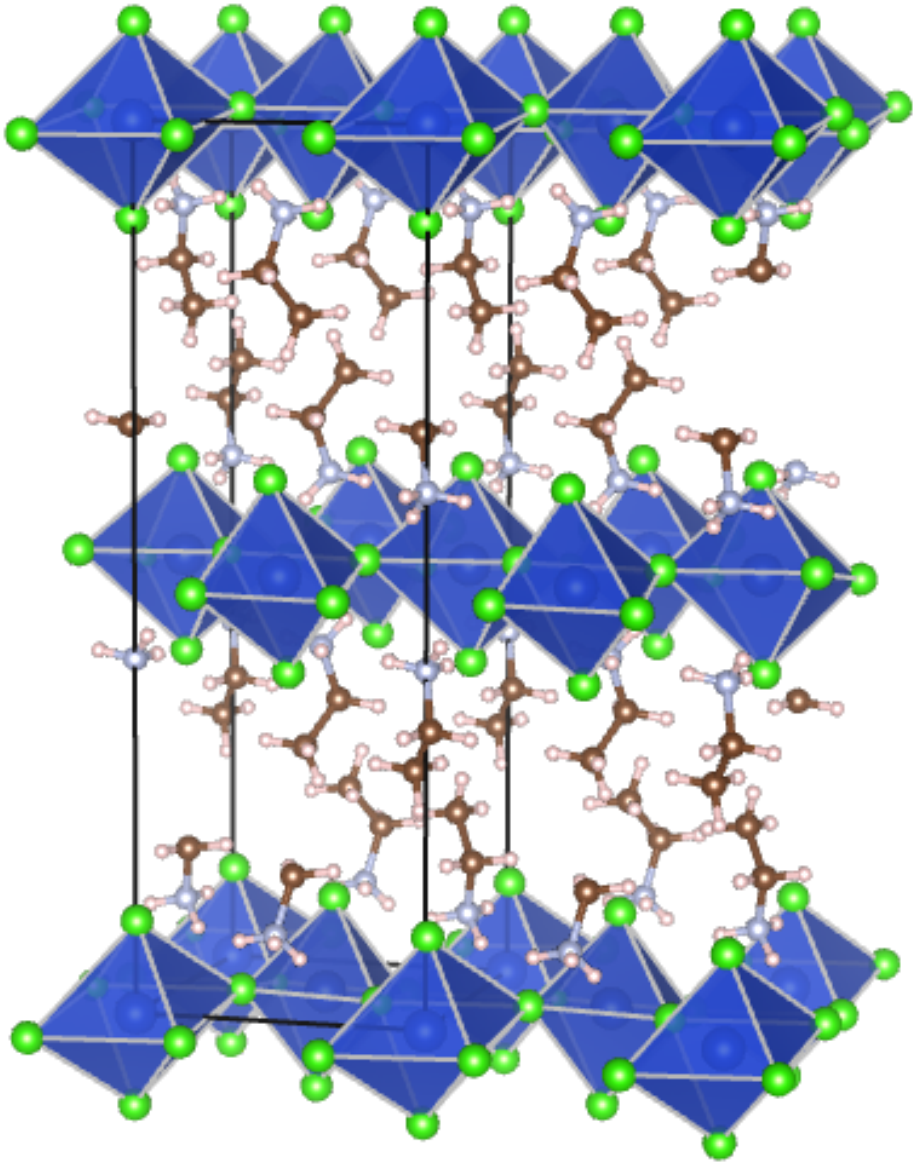
$(C_6H_5CH_2CH_2NH_3)_2[CuCl_4]$

Space group: Pbca (61)
a (Å) = 7.2099
b (Å) = 7.2664
c (Å) = 38.238

188 atoms in unit cell



# Crystal Structure of Cu-Hybrid-*EA*



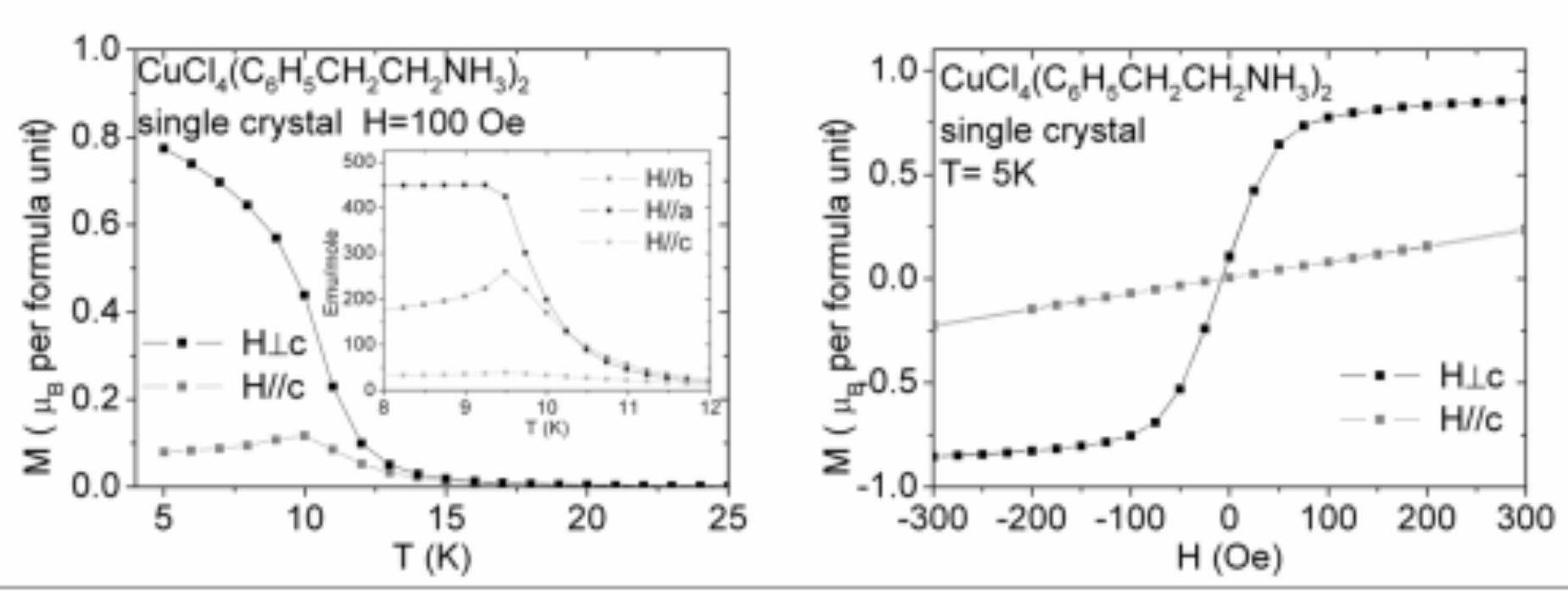
(2-Ethyl Ammonium) tetrachlorocuprate (II)

$(C_2H_5NH_3)_2[CuCl_4]$

Space group: Pbca (61)
a (Å) = 7.4789
b (Å) = 7.1713
c (Å) = 21.2406

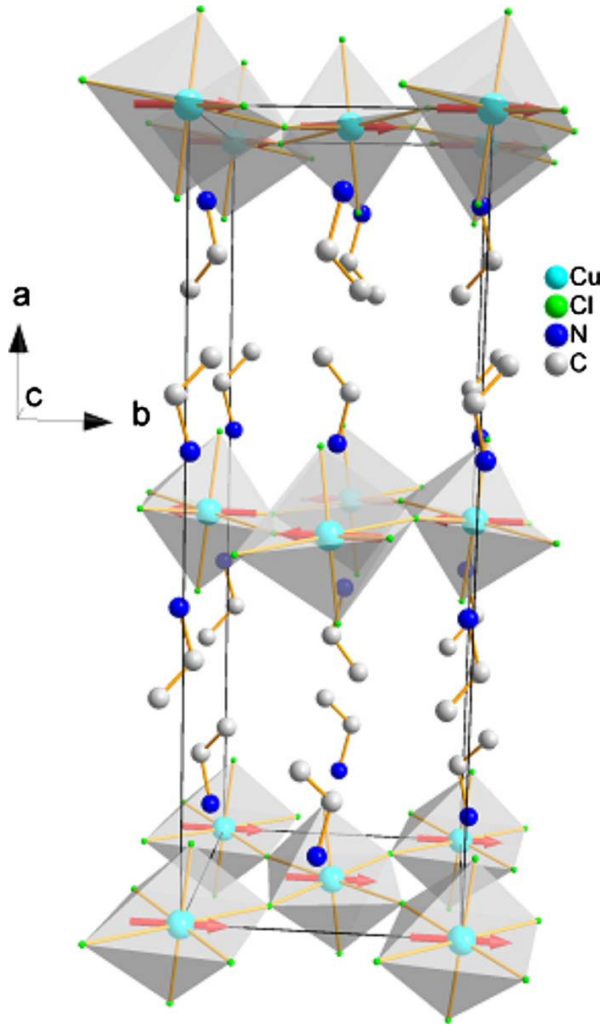
108 atoms in unit cell

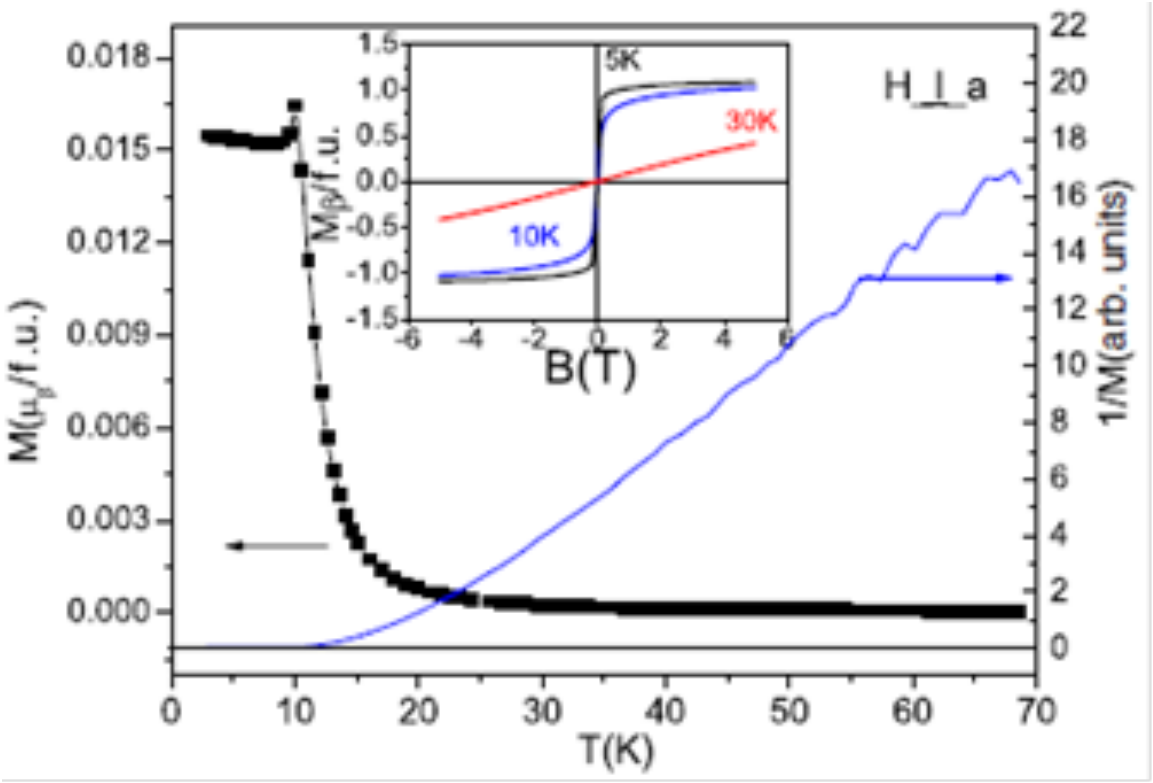
# Magnetic Properties of Cu-Hybrid-*PEA*




[A. Arkenbout, Ph.D Thesis, RuG (2010) ]

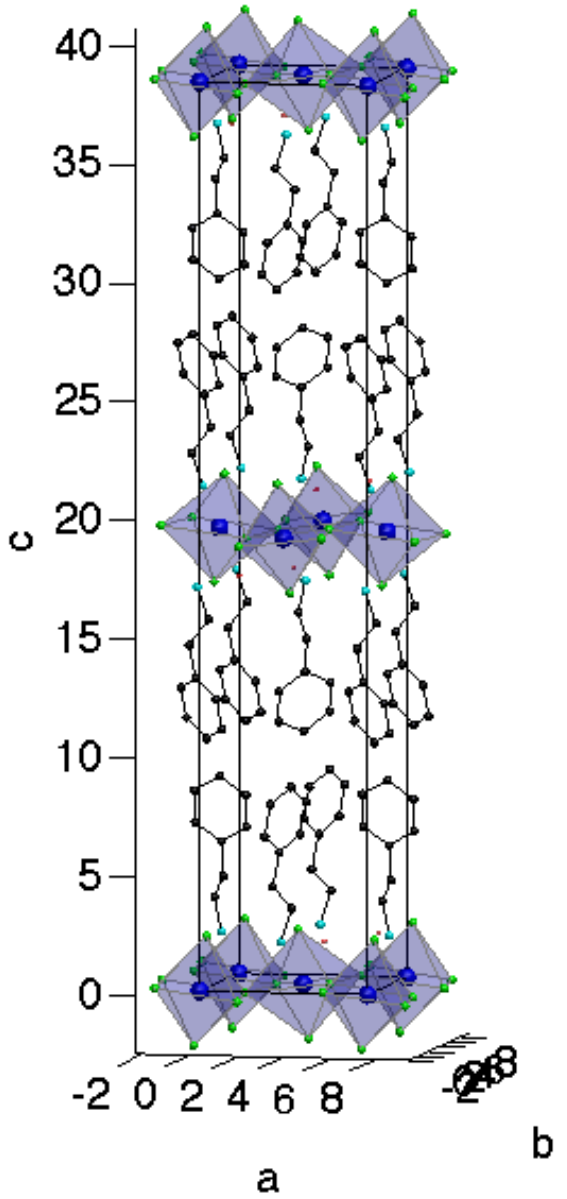
# Magnetic Properties of Cu-Hybrid-*EA*

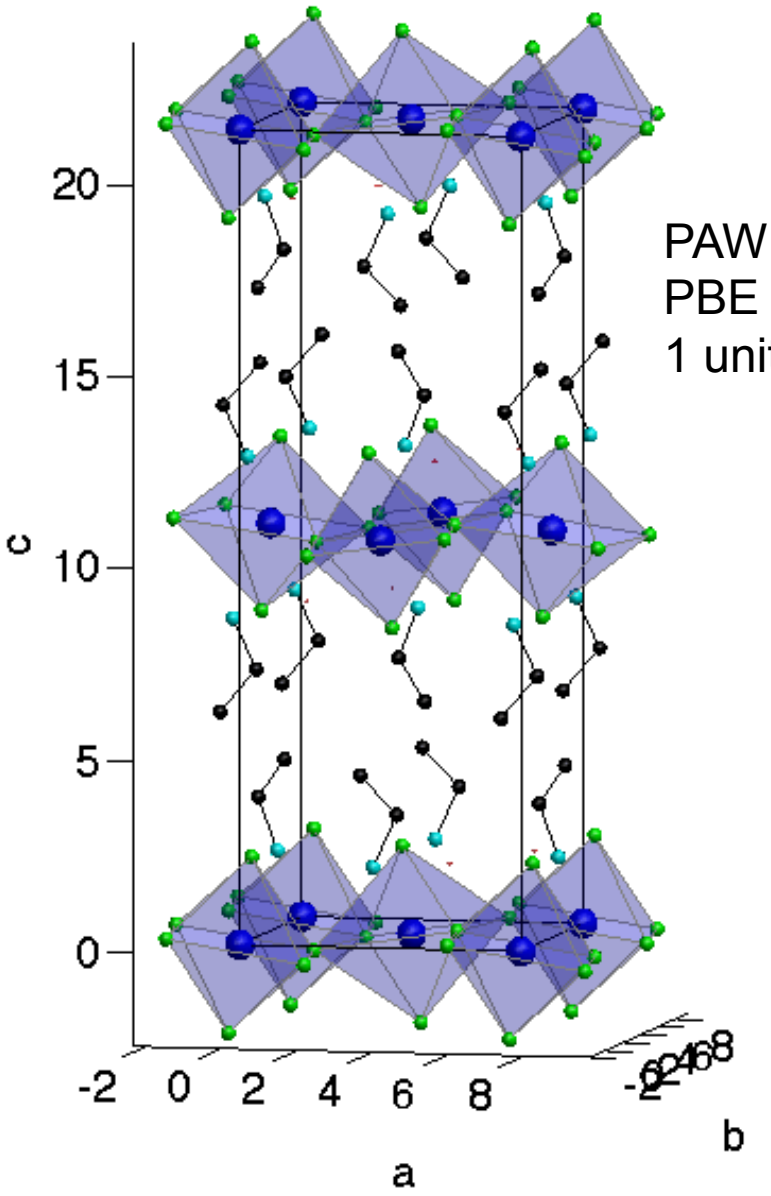



[B. Kundys, PRB **81**, 224434 (2010)]

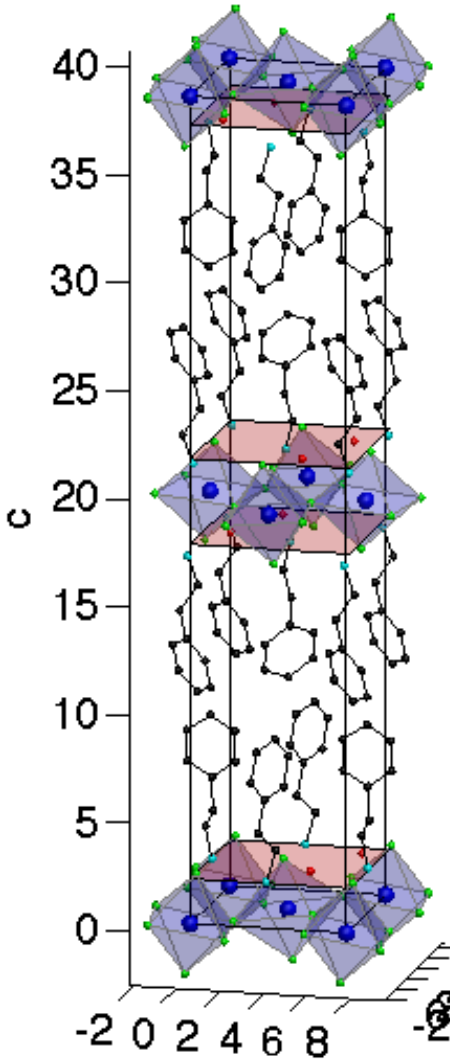
# DFT calculation by VASP

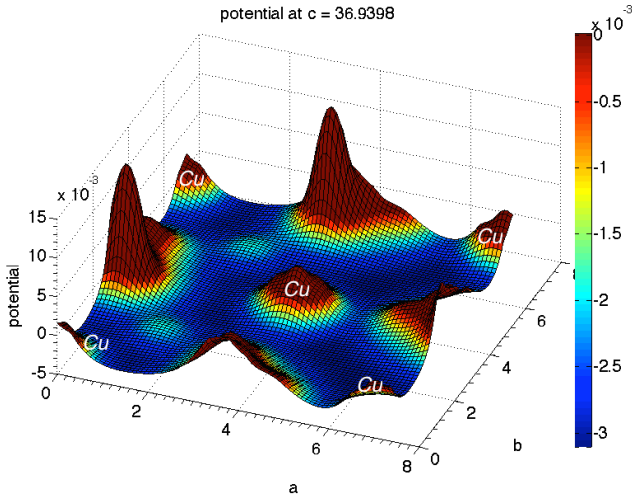


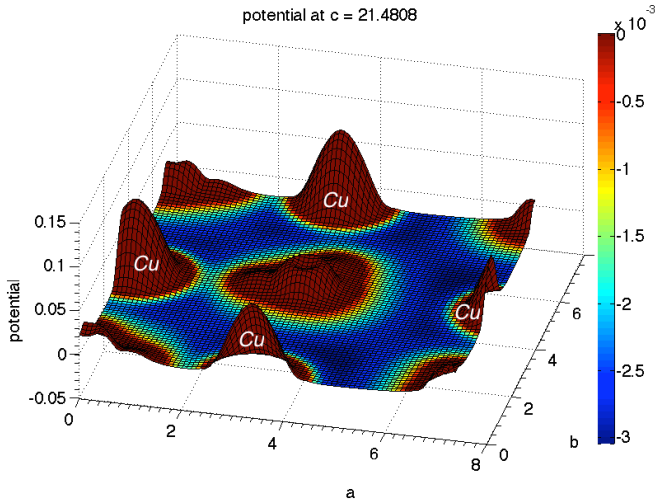



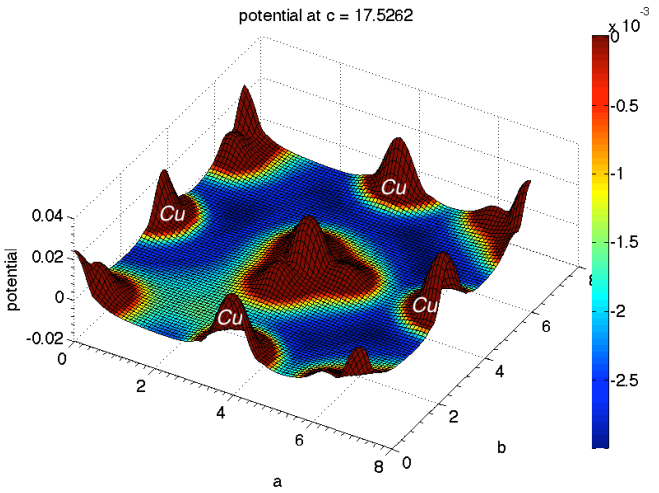

PAW DFT Calculation
PBE pseudo-potential
1 unit cell calculation

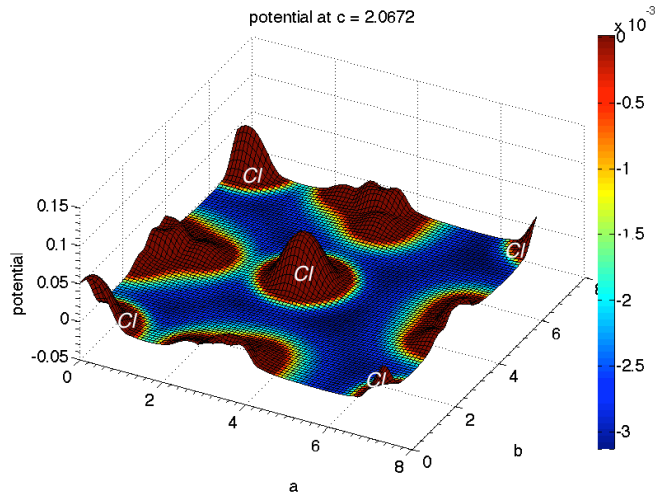
# Potential calculation on Cu-hybrid-*PEA*



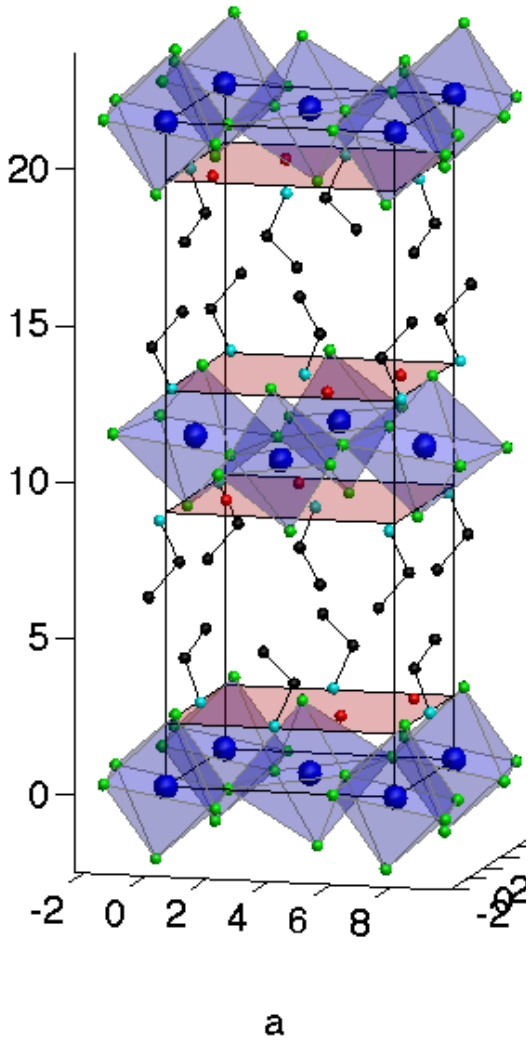



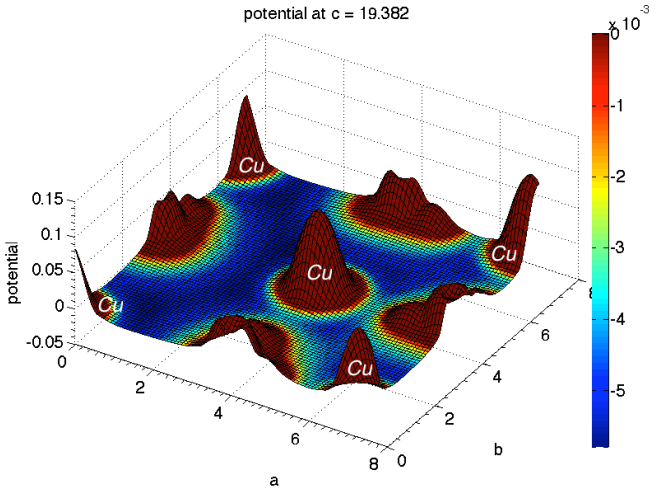



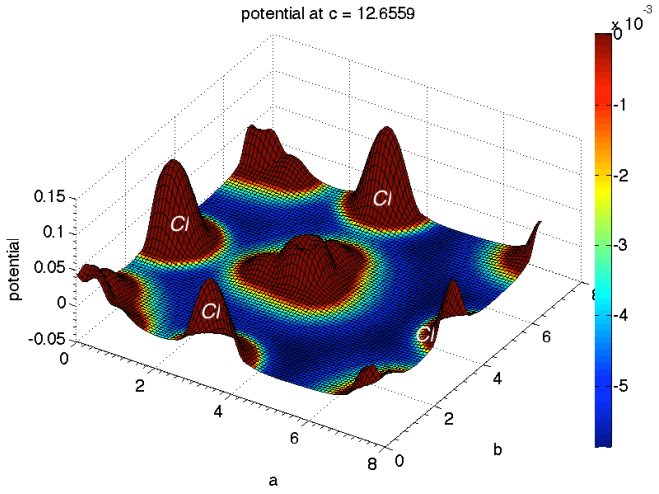



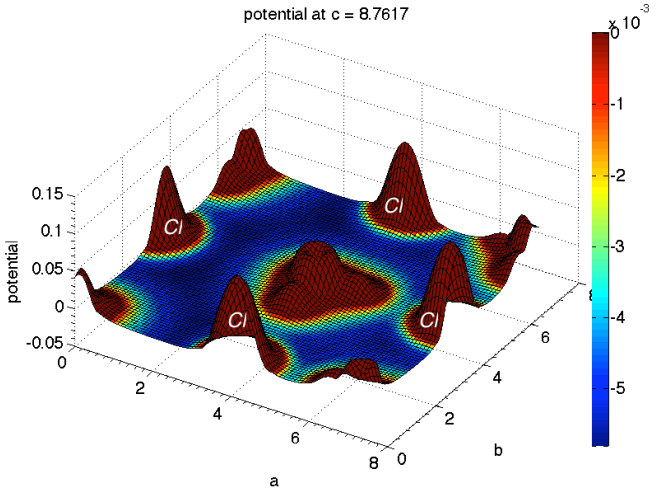



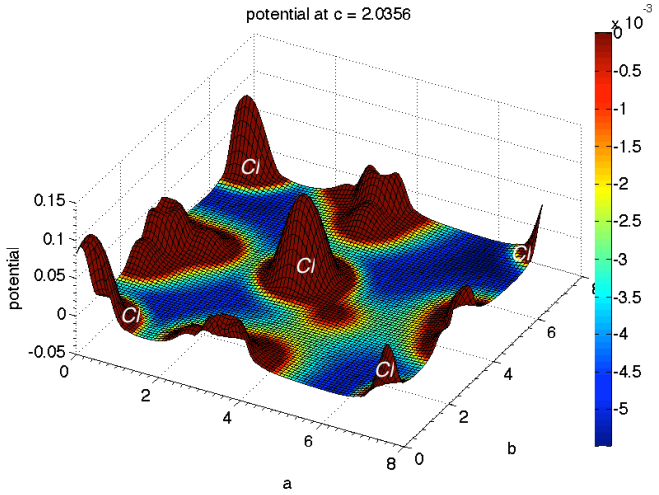
# Potential calculation on Cu-hybrid-*EA*



# Summary

- 3D magnetic ordering and the existence of strong interlayer coupling of separated 2D inorganic part about 2 nm is founded on the Hybrid materials.
- We have performed ab-initio DFT calculation on Cu-Hybrid Materials
- Muon sites position have been obtained outside the octahedral around $Cl^-$ ion
- Some additional calculations to estimate the muonium and muon positions near organic parts are going on.