



# Research Field: COSMOCHEMISTRY

## Focused Field: First-Principles Calculation

### SHORT BIO

I studied Chemistry at Nanjing University for my undergraduate and master's degrees. I honed my skills in the synthesis of compounds and the use of advanced instrumental analysis techniques. During this period, I collaborated with TCL to synthesize novel OLED materials.

Apart from my work in the lab, I also study computational calculations based on DFT, which can predict some physical properties and chemical reaction mechanisms of compounds.

I then went on to Macau University of Science and Technology to complete my PhD. and focused on first-principles computations for meteorites and mineral materials.

### Post Doctoral

**Pak-Kin Leong**  
(梁柏健)



PhD.: Earth and Planetary Science  
– Macau University of Science and Technology

M.Sc.: Chemistry – Nanjing University

B.Sc.: Chemistry – Nanjing University

### KEY PUBLICATIONS *(first author)*

**Leong Pak-Kin**, Sekine Toshimori, Tam Kuan-Vai, Tam Sok-I, and Tang Chi-Pui. 2023.  
*First-Principles Calculations with Six Structures of Alkaline Earth Metal Cyanide  $A(CN)_2$  ( $A = Be, Mg, Ca, Sr, \text{ and } Ba$ ): Structural, Electrical, and Phonon Properties.* **ACS Omega**.

**Leong Pak-Kin**, Tang Chi-Pui, Tam Sok-I, and Sekine Toshimori. 2019.  
*A DFT Study of the Structure and Properties of Nitrogen Doping Spinel  $MgAl_2O_{3.5}N_{0.5}$ .* **Meteorit. Planet. Sci.**

### PROFESSIONAL EXPERIENCE

**Ongoing – 2023** – Macau University of Science and Technology, Macao (China) – Post doctoral

**2022/11 – 2023/1** – University of Tokyo, Tokyo (Japan) – Exchange with Mikouchi group

### GRANTS

**FDTC – 2021-2023** – Participant

The cause and mechanism to accommodate certain elements in meteoritic silicates

**FDCT – 2017-2020** – Participant

Geochemical studies of Chang'e-5 lunar samples