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The Explanation of Chemical Structure

Date : 31 October 2025 (Friday)

Time : 13:30 – 14:30

Venue : LKK306 & Zoom Seminar

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Chemical structure is a key notion in chemistry and related sciences. Many chemists work on identifying structures and relating them to material properties. Successfully, using *ab initio* computational methods to model chemical structures from first principles is a key marker of cognitive scientific progress, by offering explanation and understanding. By contrast, modern deep neural network approaches, such as AlphaFold2, have achieved remarkable success in predicting complex chemical structures, without explicitly including theories of chemistry or physics. Thus, they do not contribute to scientific progress in the same way.

This paper explores the first aspect of that argument. I turn to well-known theories of scientific explanation to see whether chemical structures can be explained from first principles. I show that this is possible, but that, depending on the complexity and nature of the *explanandum*, we need to be pragmatic by drawing on aspects of different theories of scientific explanation.

All are welcome

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