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How To Avoid Optimising Molecular Geometry

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ABSTRACT

We may never be able to fully understand how matter behaves at the molecular level. It is reasonable to suppose that there are some phenomena, and some theories which might in principle be devised, which are so complex that they are likely to always be beyond human comprehension. The detailed description of molecular behaviour may well fall into that category.

If we do not really understand what is happening between molecules, one might argue that this lessens the importance of calculating exact molecular properties (is there perhaps some ambiguity in what we mean by “exact” in this context?).

Nevertheless, there are good reasons why it is still desirable to determine molecular parameters to the highest possible accuracy. A precise description of a molecule’s structure is a powerful test of the theory used to derive that structure. Knowledge of molecular shape is also of central importance in practical fields such as computational drug design, in which the potential of candidate drugs is related to the degree to which they fit into – and interact with – the active site of target proteins.

Molecular optimization, however, does not invariably imply the determination of the exact geometry of one particular molecule. We can also apply the term to the identification of the approximate geometry of a candidate molecule from a pool containing many thousands or millions of molecules. This process is, in a sense, optimization of properties rather than of structure, but as “structure” is one of those properties, it is clear that the two tasks are closely linked.

In this talk I will discuss the potential of Artificial Intelligence (AI) methods in tackling property optimization tasks. We shall see that the process of seeking out a molecule with exceptional properties from a large candidate pool has much in common with that of optimizing molecular structure.