

What I learned about structure from artificial intelligence

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We sometimes wonder what artificial intelligence can teach us that we don't already know. Are there important life-lessons that we can glean from our interactions with AI beyond a more efficient (and more error prone) web search?

In my case, the answer is a firm yes, but in a slightly surprising way. I have been a "crystallographer" (the quotes are because I like structure beyond crystals) for my whole long career and for the entire time, whilst often advocating for looking beyond the crystallographic description of structure, I have never questioned my understanding of what a structure is.

However, when thinking about how to use AI and machine learning (ML) to study structure, new questions were brought into sharp focus that questioned my very understanding of what a structure is.

In this talk I will share this intellectual journey. The journey is not over and I hope that interaction with natural intelligence (the audience members) can help to move the journey forward. I believe that there are somewhat serious and interesting implications for the large and growing industry of people applying ML to materials discovery.