Materials Design in the Information Age and Beyond

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Materials discovery has been greatly accelerated by techniques of artificial intelligence in the modern Information Age. But we are also expecting critical challenges from big materials data to computationally intense machine learning processes, as Moore's law is coming to an end. Quantum computers, which use quantum superposition and interference to perform computations, hold great potential in handling big data and accelerating the optimization algorithms ubiquitous in machine learning models. As more and more quantum bits become available, the dawn of the Quantum Age is approaching us at speed. In this talk, I will use a new family of materials called high-entropy materials (HEMs) as an example to demonstrate how classical and quantum computers join forces to discover new HEMs that exhibit excellent properties, and to prepare for the upcoming challenges in materials discovery.

References:

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