Expanding the horizon of automated metamaterials discovery via quantum annealing

Koji Tsuda[a,b,c]

[a] *University of Tokyo,* [b] *NIMS,* [c]*RIKEN AIP*
tsuda@k.u-tokyo.ac.jp

Complexity of materials designed by machine learning is currently limited by the inefficiency of classical computers. We show how quantum annealing can be incorporated into automated materials discovery and conduct a proof-of-principle study on designing complex thermofunctional metamaterials consisting of SiO2, SiC, and Poly(methyl methacrylate). The difficulty of this black-box optimization problem grows exponentially in the number of variables. Our quantum-classical hybrid algorithm consists of a factorization machine, an atomistic simulator, and a D-Wave 2000Q quantum annealer. Apart from the computational time needed for simulation, quantum annealing reduced the processing time to near zero regardless of the problem size. Our method was used to design complex structures of wavelength selective radiators showing much better concordance with the thermal atmospheric transparency window in comparison to existing human-designed alternatives. This result shows that quantum annealing can be used effectively in real-world design problems and indicates the direction of further applications.

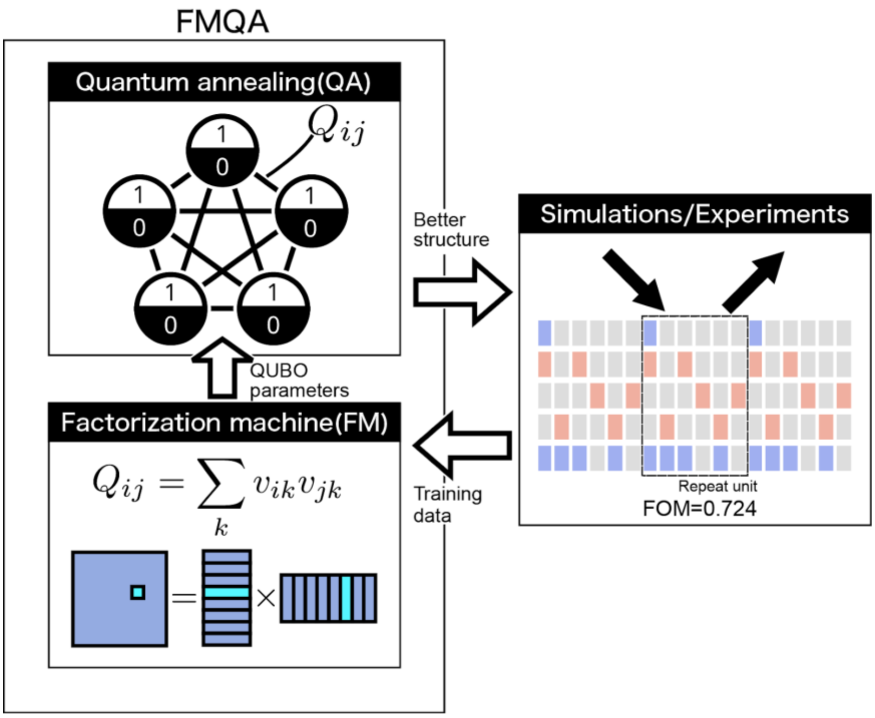

Figure 1: Procedure of our automated materials discovery using a factorization machine (FM) for learning and a quantum annealer (QA) for selection. Target property is the figure-of-merit (FOM) for the radiative sky cooling, which is evaluated by the rigorous coupled wave analysis (RCWA).

References

1. K. Kitai, J. Guo, S. Ju, S. Tanaka, K. Tsuda, J. Shiomi, and R. Tamura, Expanding the horizon of automated metamaterials discovery via quantum annealing, arXiv, 1902.06573, 2019