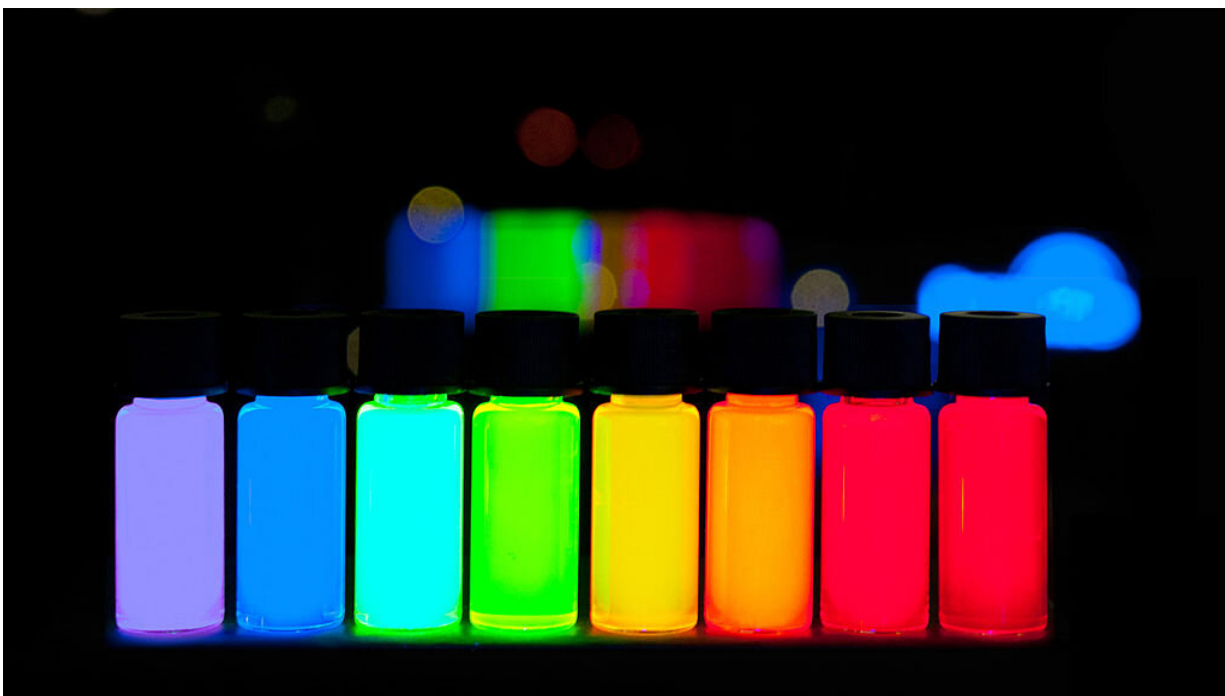# A machine learning solution for designing materials with desired optical properties

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Controlling light-matter interactions is central to a variety of important applications, such as quantum dots, which can be used as light emitters and sensors. Credit: PlasmaChem

Understanding how matter interacts with light—its optical properties—is critical in a myriad of energy and biomedical technologies, such as targeted drug delivery, quantum dots, fuel combustion, and cracking of biomass. But calculating these properties is computationally intensive,

and the inverse problem—designing a structure with desired optical properties—is even harder.

Now Berkeley Lab scientists have developed a machine learning model that can be used for both problems—calculating optical properties of a known structure and, inversely, designing a structure with desired optical properties. Their study was published in *Cell Reports Physical Science*.

"Our model performs bi-directionally with high accuracy and its interpretation qualitatively recovers physics of how metal and dielectric materials interact with light," said corresponding author Sean Lubner.

Lubner notes that understanding radiative properties (which includes optical properties) is equally important in the natural world for calculating the impact of aerosols such as black carbon on climate change.

The machine learning model proposed in this study was trained on spectral emissivity data from nearly 16,000 particles of various shapes and materials that can be experimentally fabricated.

"Our machine learning model speeds up the inverse design process by at least two to three orders of magnitude as compared to the traditional method of inverse design," said co-author Ravi Prasher, who is also Berkeley Lab's Associate Director for Energy Technologies.

Mahmoud Elzouka, Charles Yang, and Adrian Albert, all scientists in Berkeley Lab's Energy Technologies Area, were also co-authors.

More information: Mahmoud Elzouka et al, Interpretable Forward and Inverse Design of Particle Spectral Emissivity Using Common Machine-Learning Models, *Cell Reports Physical Science* (2020). DOI: 10.1016/j.xcrp.2020.100259

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