

# Plasmonic Nanoparticle Simulation and Inverse Design Using Machine Learning

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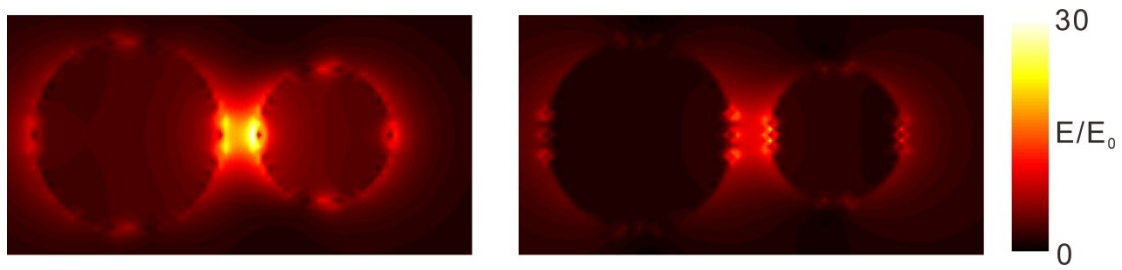
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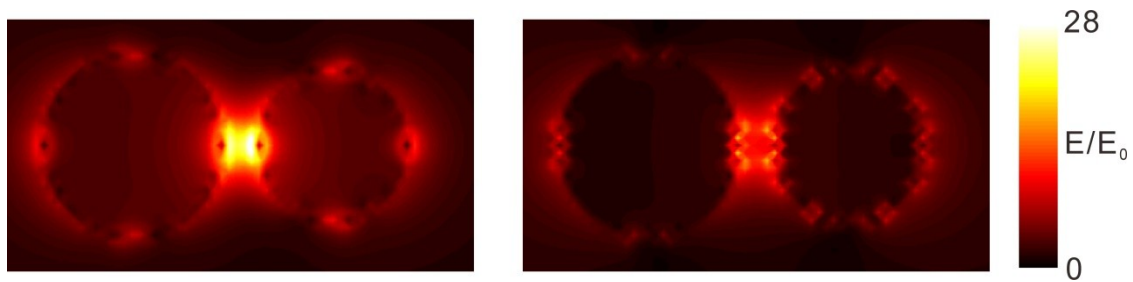
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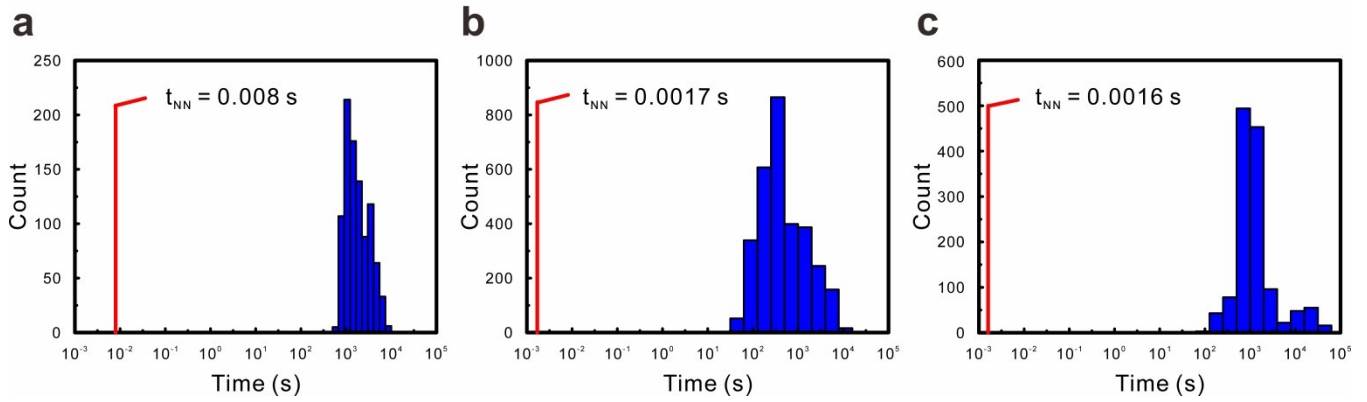
**Figure S1.** Comparison of the electric-field enhancement distributions of dimer (34/24/7) at the (left) dipolar (542 nm) and (right) coupling (618 nm) modes.



**Figure S2.** Comparison of the electric-field enhancement distributions of dimer (24/20/5) at the (left) dipolar (542 nm) and (right) coupling (613 nm) modes.



**Figure S3.** Comparison of the electric-field enhancement distributions of dimer (38/26/1) at the (left) dipolar (532 nm) and (right) coupling (637 nm) modes.



**Figure S4.** Comparisons of the time consumed by numerical simulation and machine learning of Au (a) NSs, (b) NRs, and (c) NS dimers. The blue histograms show the time costed by performing the FDTD simulations on a server (16 cores and 64 GB RAM) and the red lines label the time costed by performing the machine learning process (2 cores and 8 GB RAM).