

## Supporting Information

for

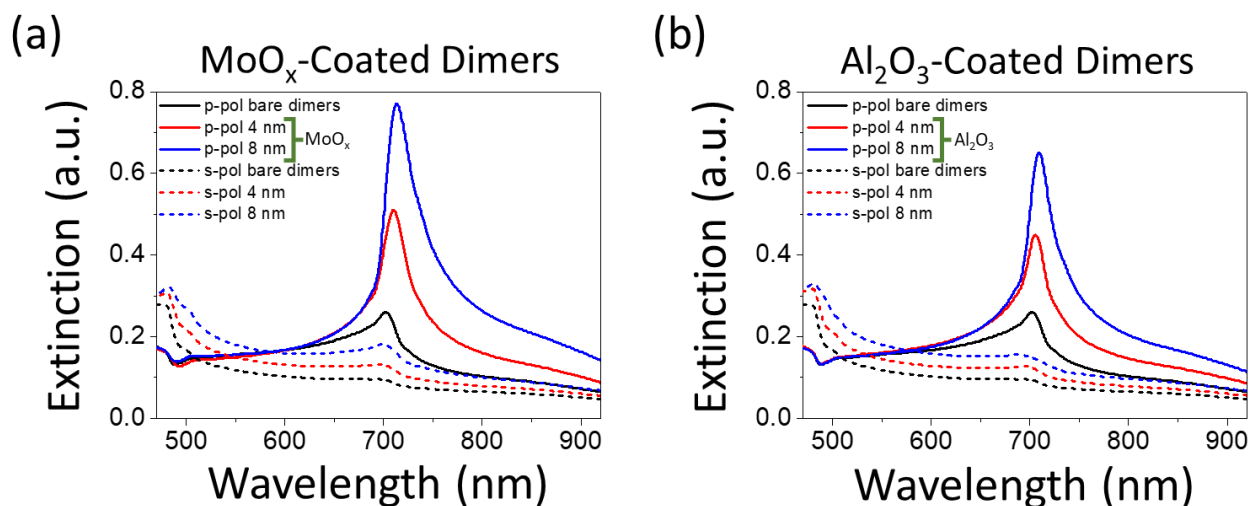
# Molybdenum Oxide Functional Passivation of Aluminum Dimers for Enhancing Optical-Field and Environmental Stability

Daniela Lorenzo <sup>1,\*</sup>, Fabrizio Riminucci <sup>2</sup>, Mariachiara Manoccio <sup>1</sup>, Gianluca Balestra <sup>1</sup>, Daniela Simeone <sup>1</sup>, David Maria Tobaldi <sup>1</sup>, Marco Esposito <sup>1</sup>, Adriana Passaseo <sup>1</sup>, Vittorianna Tasco <sup>1</sup> and Massimo Cuscunà <sup>1,\*</sup>

1 CNR NANOTEC Institute of Nanotechnology, Via Monteroni, Lecce 73100, Italy; daniela.lorenzo@nanotec.cnr.it (D.L.); mariachiara.manoccio@unisalento.it (M.M.); gianluca.balestra@nanotec.cnr.it (G.B.); daniela.simeone@nanotec.cnr.it (D.S.); david.tobaldi@nanotec.cnr.it (D.M.T.); marco.esposito@nanotec.cnr.it (M.E.); adriana.passaseo@nanotec.cnr.it (A.P.); vittorianna.tasco@nanotec.cnr.it (V.T.); massimo.cuscuna@nanotec.cnr.it (M.C.)

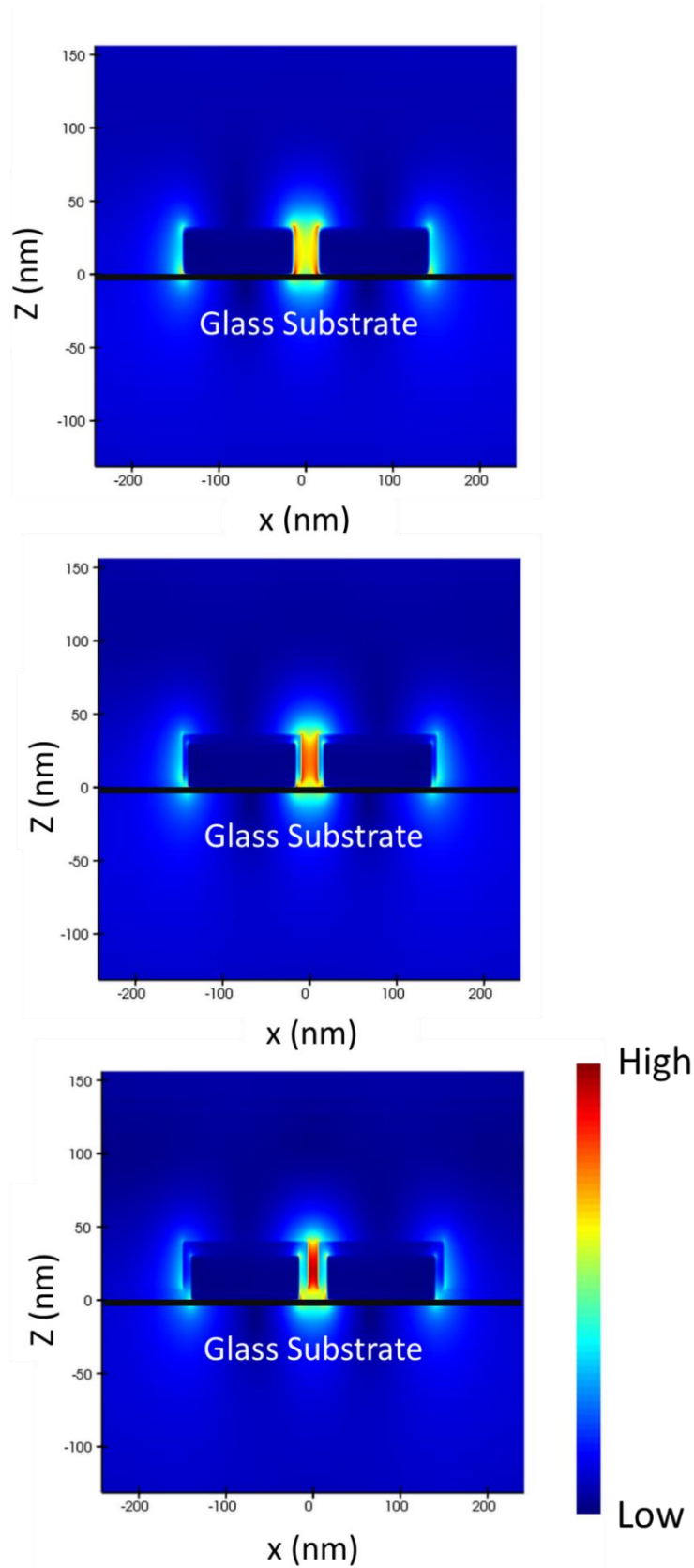
2 Molecular Foundry, Lawrence Berkeley National Laboratory, One Cyclotron Road, Berkeley 94720, CA, United States; fabrizioriminucci@lbl.gov (F.R.)

\* Correspondence: [massimo.cuscuna@nanotec.cnr.it](mailto:massimo.cuscuna@nanotec.cnr.it); [daniela.lorenzo@nanotec.cnr.it](mailto:daniela.lorenzo@nanotec.cnr.it)

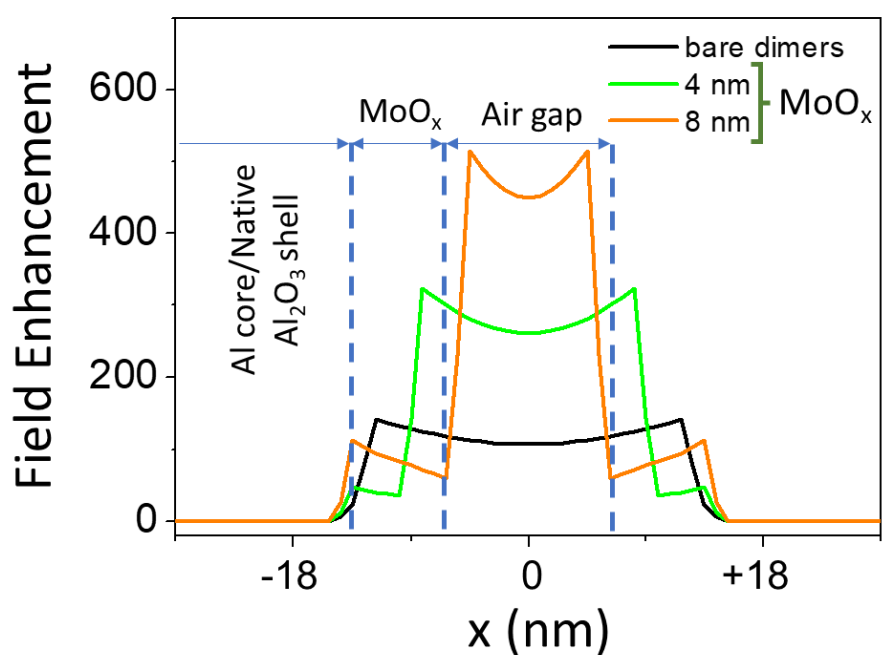


**Figure S1.** Simulated extinction spectra for Al dimers by progressively increasing the (a) MoO<sub>x</sub> and (b) Al<sub>2</sub>O<sub>3</sub> coatings on bared Al nanostructures (Al core/native Al<sub>2</sub>O<sub>3</sub> shell dimers) up to 4 and 8 nm thick dielectric films, for s-pol and p-pol polarized excitation.

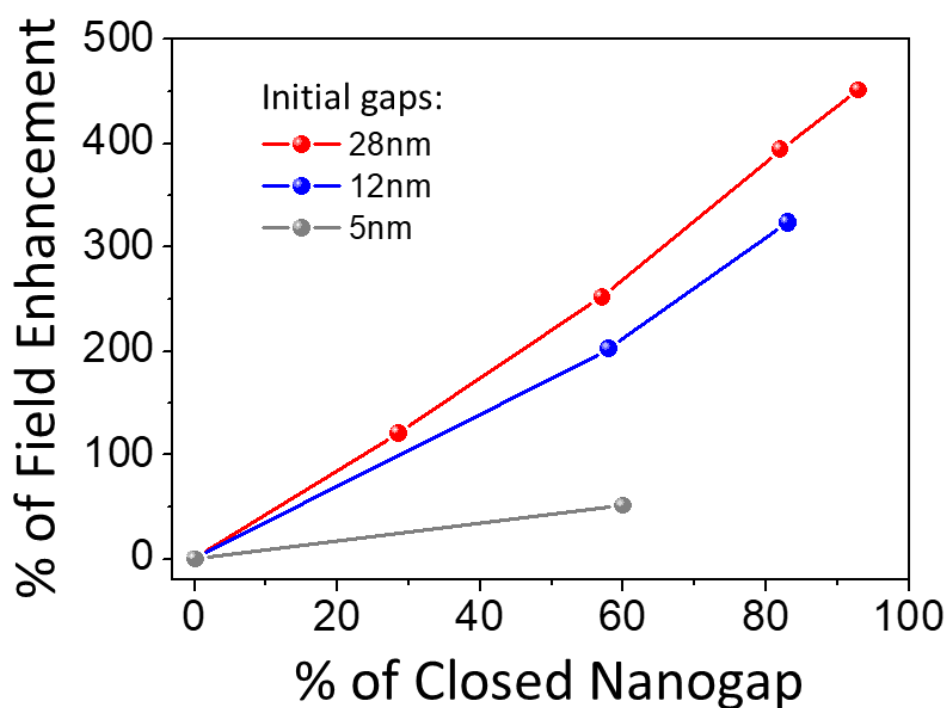
Figure S1 demonstrates the beneficial role of the dielectric coating, which provides an enhanced optical extinction, for longitudinal polarized excitation, by increasing the oxide thickness. Such an increase in the extinction is larger for high refractive index oxide coating as MoO<sub>x</sub>, with respect to the Al<sub>2</sub>O<sub>3</sub> film.



**Figure S2.** Calculated two-dimensional near-field enhancement factor  $|E/E_0|^2$  ( $E_0 = 1 \text{ V/m}$ ) maps (side view) for the bare (Al core/native  $\text{Al}_2\text{O}_3$  shell dimers) and coated dimers with  $\text{MoO}_x$  layers (4 and 8 nm thick films). The maps are extracted at corresponding wavelengths of maximum extinction peaks reported in Figure 2a (right panel), and at the nanoantenna height where the EM field is maximum.



**Figure S3.** Simulated variations of field enhancement ( $|E/E_0|^2$ ) values across the nanogap of the bare and coated dimers reported in Figure S2. The field enhancement was extracted at the nanoantenna height where the EM field is maximum.



**Figure S4.** Percentage of EM field enhancement as function of the percentage of narrowed gap (by  $\text{MoO}_x$  ALD deposition), with respect to bare dimers for three initial nanogaps of 28, 12 and 5 nm.