# Supplementary Information

## Enhanced Electrochemical Activity of MgO Nanoparticles for High-Performance Supercapacitors

Megha Goyal,[a] Sarvesh Kumar Pandey,[b*] and Nitu Bhatnagar[a*]

[a]Department of Chemistry, Manipal University Jaipur, Jaipur – 303007, Rajasthan (India)

[b]Department of Chemistry, Maulana Azad National Institute of Technology Bhopal, Bhopal - 462003, Madhya Pradesh (India)

Corresponding Authors' Email
E-mail: sarvesh@manit.ac.in
niturbhatnagar@gmail.com

**Table S1.** Some Selected and Useful Parameters of the MgONPs using the DFT Approach

| **Parameter** | **Calculated Value** |
|---|---|
| Dipole moment (Debye) | 7.3 |
| Electronic energy (Hartree) | -4131.404 |
| $E_{HOMO}$ (eV) | -4.068 |
| $E_{LUMO}$ (eV) | -10.639 |
| Ionization potential, $I = -E_{HOMO}$ | 4.068 |
| Electron affinity, $A = E_{LUMO}$ | 10.639 |
| Energy gap, $\Delta E = E_{LUMO} - E_{HOMO}$ | -6.571 |
| Electronegativity, $\chi = (I + A)/2$ | 7.353 |
| Hardness, $\eta = (I-A)/2$ | -3.285 |
| Softness ($eV^{-1}$), $\sigma = 1/\eta$ | -0.304 |
| Electrophilicity, $\omega = \mu^2/2\eta$ | -8.229 |
| Nucleophilicity, $\varepsilon = 1/\omega$ | -0.121 |
| Total energy change of back-donation, $\Delta E_{b-d} = -\eta/4$ | 0.821 |
| Electron accepting power, $\omega^+ = (I + 3A)^2/16(I - A)$ | -12.317 |
| Electron donating power, $\omega^- = (3I + A)^2/16(I - A)$ | -4.963 |
| Net electrophilicity, $(\Delta\omega\pm) = \omega^+ + \omega^-$ | -18.279 |

**Table S2.** Energy and Power Density at Different Current Densities for the 3-Electrode Method

| **Current density (A/g)** | **Energy density (Wh/kg)** | **Power density (W/kg)** |
|---|---|---|
| 0.1 | 1.38 | 49.4 |
| 0.2 | 1.08 | 73.4 |
| 0.3 | 1.04 | 98.2 |
| 0.6 | 0.67 | 196.4 |
| 1 | 0.55 | 293.1 |
| 1.3 | 0.48 | 394.9 |
| 1.6 | 0.42 | 486.1 |
| 2.6 | 0.31 | 773.5 |
| 3.3 | 0.27 | 966.9 |

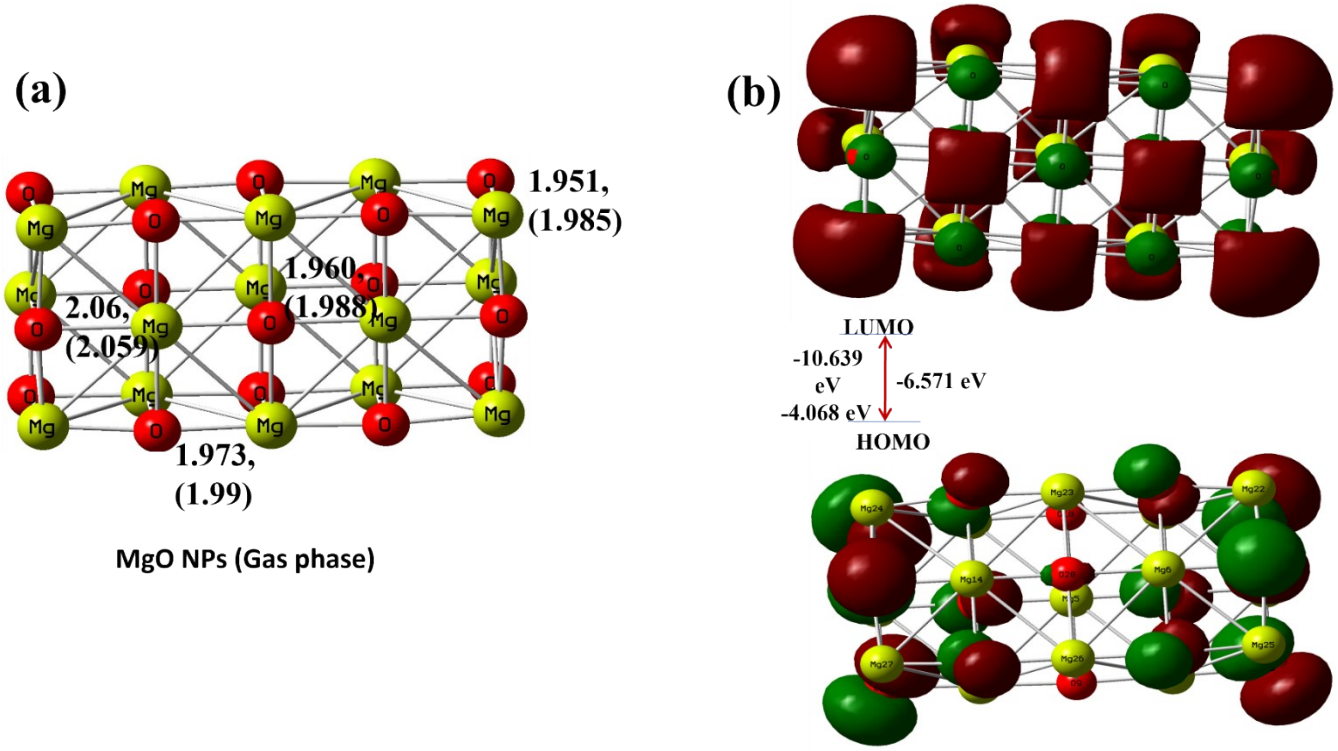


**Figure S1**. Representation of a) Optimized Structure, b) HOMOs, and LUMOs of the MgONPs

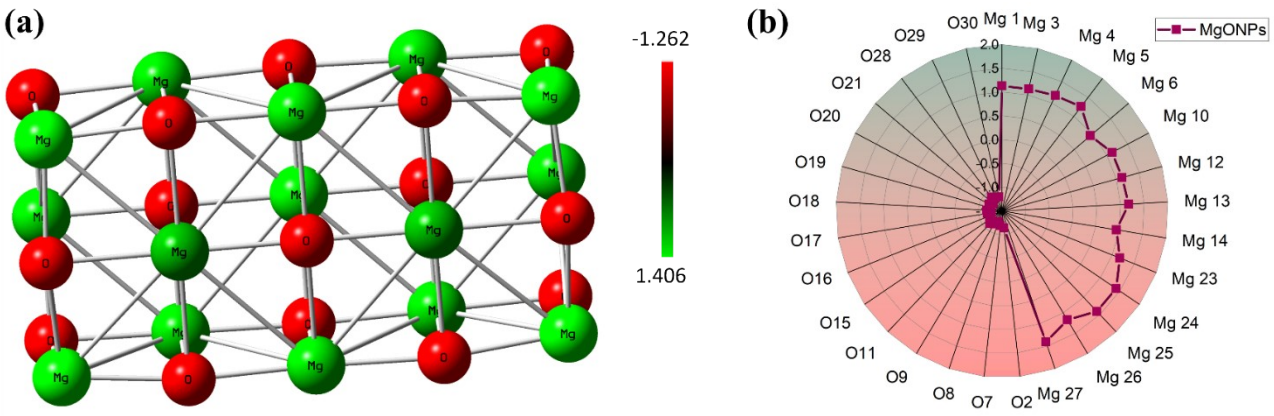


**Figure S2.** (a) Crystal structure of MgO, showing Mg (green) and O (red) atoms in a cubic arrangement. (b) Radar chart of Mulliken charges for Mg and O atoms in the structure, with

radial distance indicating charge magnitude and color gradient from red (negative) to green (positive)

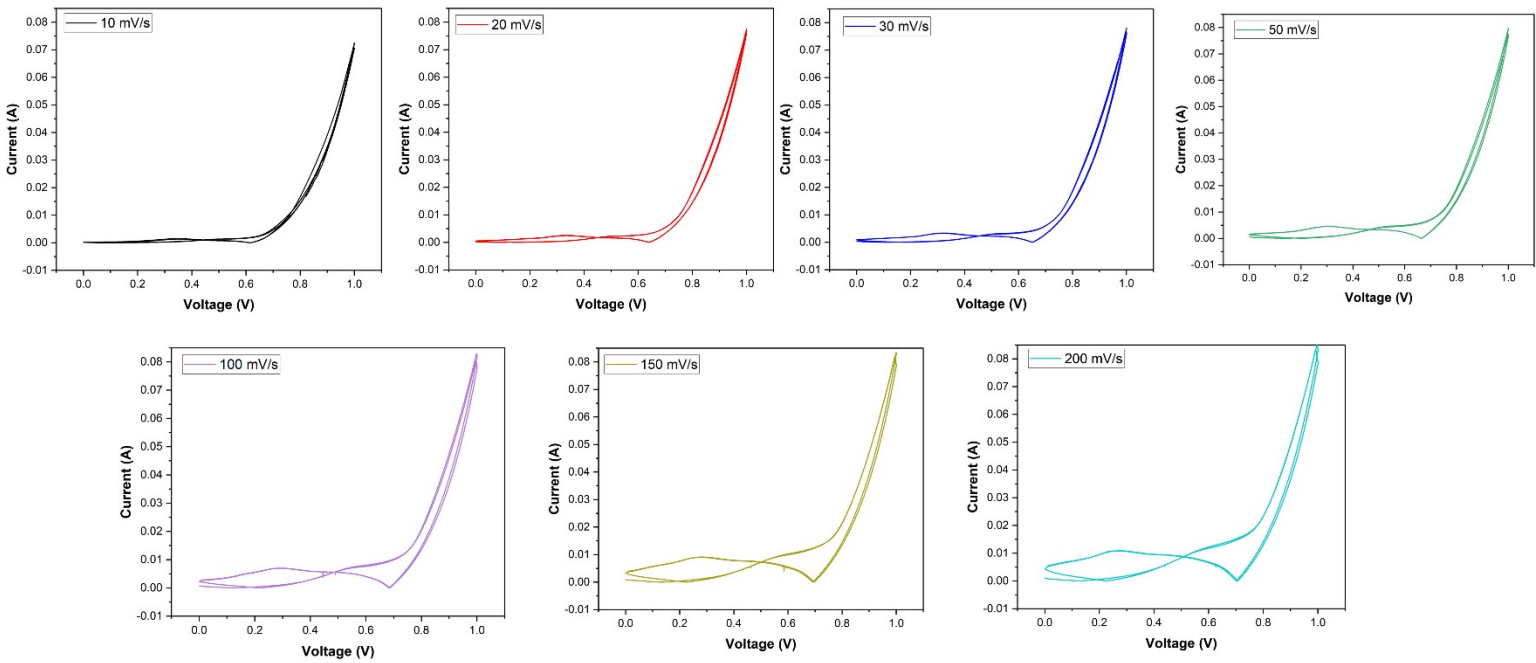


**Figure S3.** Individual CV curves of MgONPs electrodes at different sweep rates (10 to 200 $mVs^{-1}$)

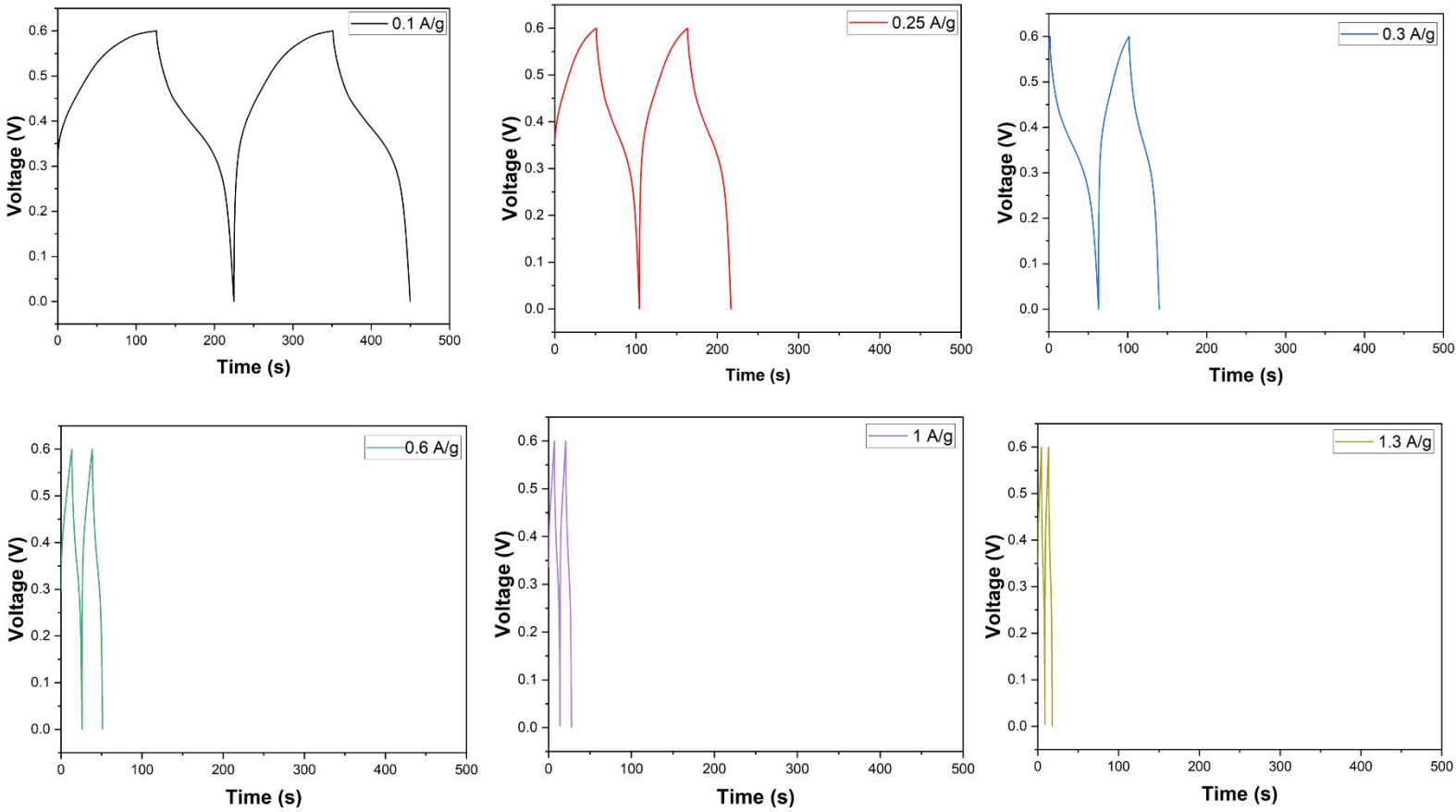


**Figure S4.** Individual GCD curves of MgONPs electrodes at different current densities (0.1 to 1.3 A/g)