

SUPPLEMENTARY INFORMATION

for

Self-Healing in Dielectric Capacitors: a Universal Method to Computationally Rate Newly Introduced Energy Storage Designs

Nadezhda A. Andreeva¹ and Vitaly V. Chaban²

(1) Peter the Great St. Petersburg Polytechnic University, Saint Petersburg, Russia.

(2) Yerevan State University, Yerevan, 0025, Armenia. E-mail: vvchaban@gmail.com

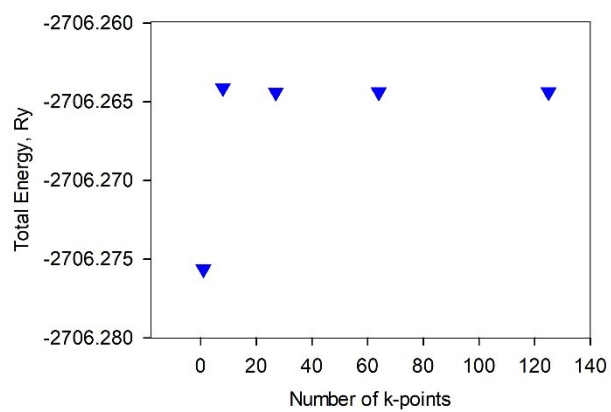


Figure S1. The total energy as of the system a function of the total number of k-points sampled. The PP + 4 Zn system was used to perform the depicted benchmark.

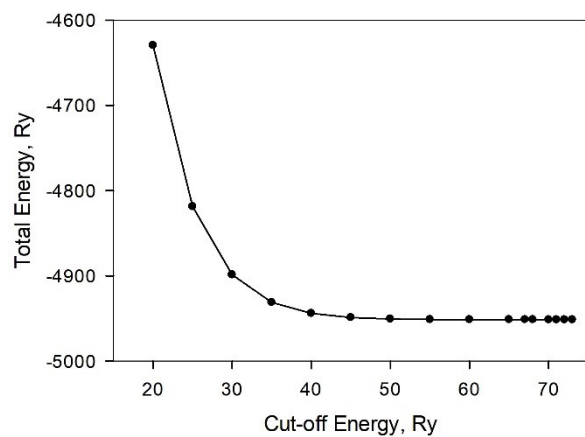


Figure S2. The total energy of the system as a function of the chosen plane-wave cut-off energy. The PP + 4 Zn system was used to perform the depicted benchmark.

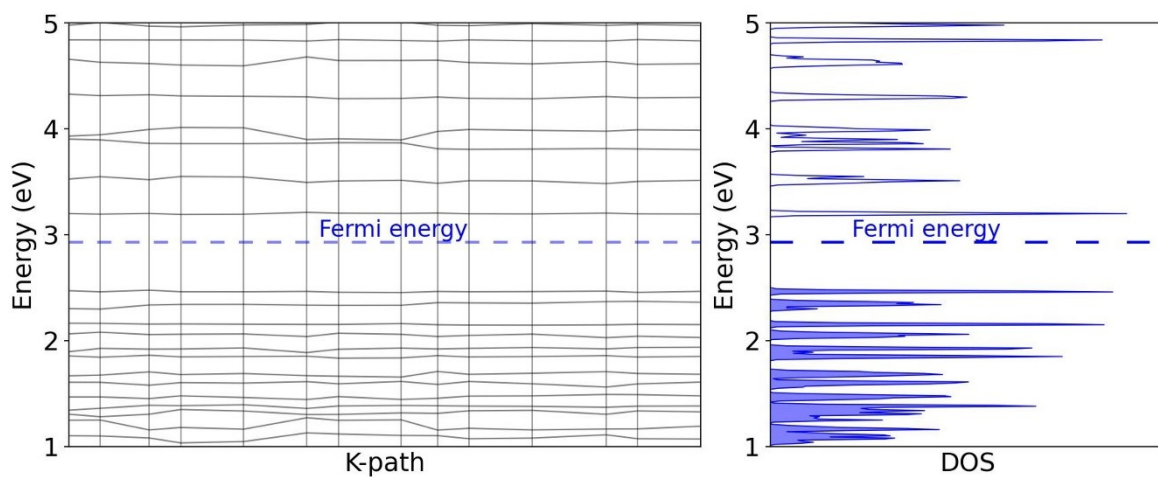


Figure S3. The band structure (left) and DOS (right) of the [4 Zn + PET] system. The band gap amounts to 0.7 eV. The Fermi energy equals 2.9 eV.

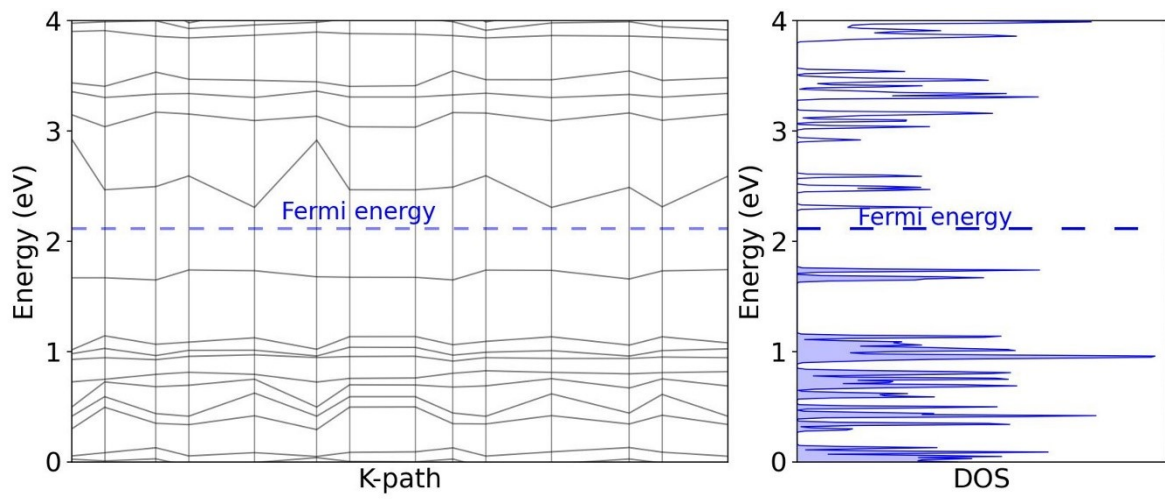


Figure S4. The band structure (left) and DOS (right) of the [4 Zn + PC] system. The band gap is 0.6 eV. The Fermi energy is 2.2 eV.

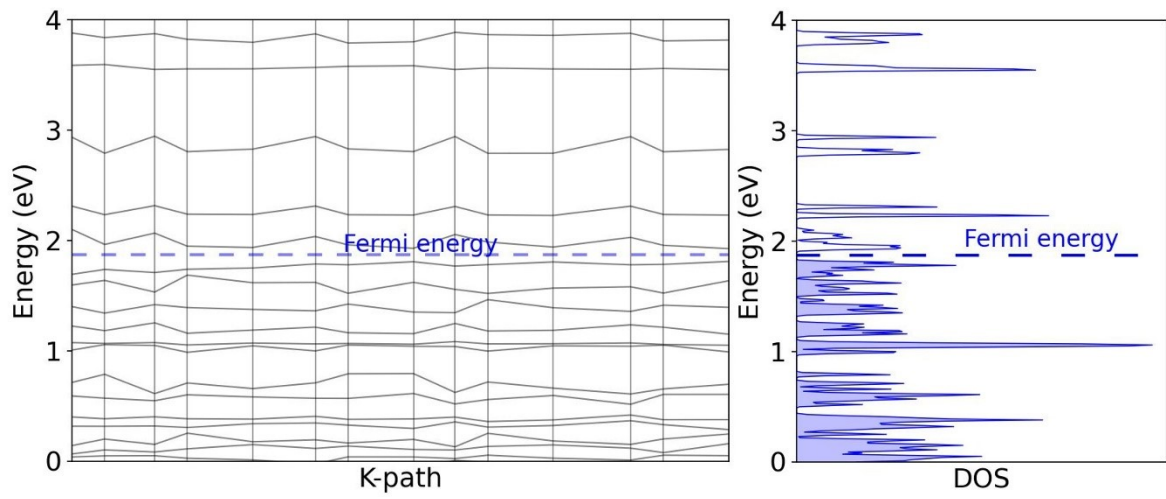


Figure S5. The band structure (left) and DOS (right) of the [4 Zn + Kapton] system. The band gap amounts to 0.12 eV. The Fermi energy is 1.9 eV.