Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information to:

Early stages in the degradation of Metal-Organic Frameworks in liquid water from first-principles Molecular Dynamics

Luca Bellarosa,[a] Sofía Calero,[b*] and Núria López[a*]

[a] *Institute of Chemical Research of Catalonia, ICIQ, Av. Països Catalans 16, 43007 Tarragona, Spain;*

[b] *Department of Physical, Chemical and Natural systems, University Pablo de Olavide, Ctra. de Utrera km. 1, 41013 Seville, Spain*

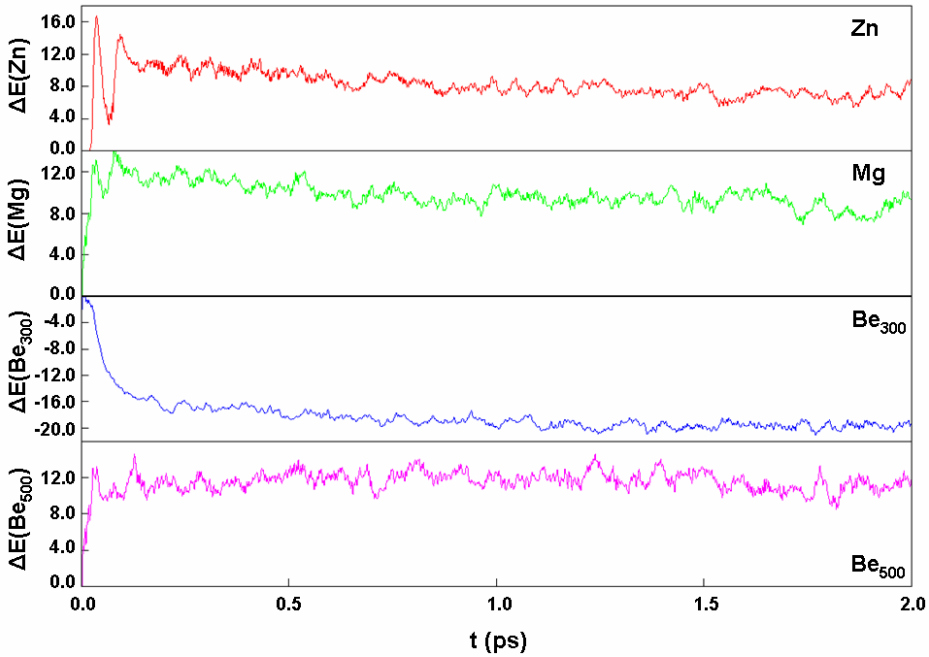

Figure S1. Potential energies for the different M-IRMOF-1 in the first two ps of simulation (equilibration time), with M=Zn, Mg, Be (T=300 K), or Be (T=500 K). All the energies, ΔE, refer to the initial configuration and are in eV. All the initial configurations were minimized; the Be_{300} case is a particular case characterized by a local minimum. All the energies oscillate around a constant value after 0.8-1.0 ps. Be_{500}, run at higher temperature, is characterized by greater oscillations.