Electronic Supplementary Material (ESI) for RSC Advances

SUPPORTING INFORMATION

Direct Ab-Initio Molecular Dynamics (MD) Study on the Ionization of Benzene Dimer

Hiroto TACHIKAWA

Division of Materials Chemistry, Graduate School of Engineering,

Hokkaido University, Sapporo 060-8628, JAPAN

1. Spin density on benzene dimer cation

.

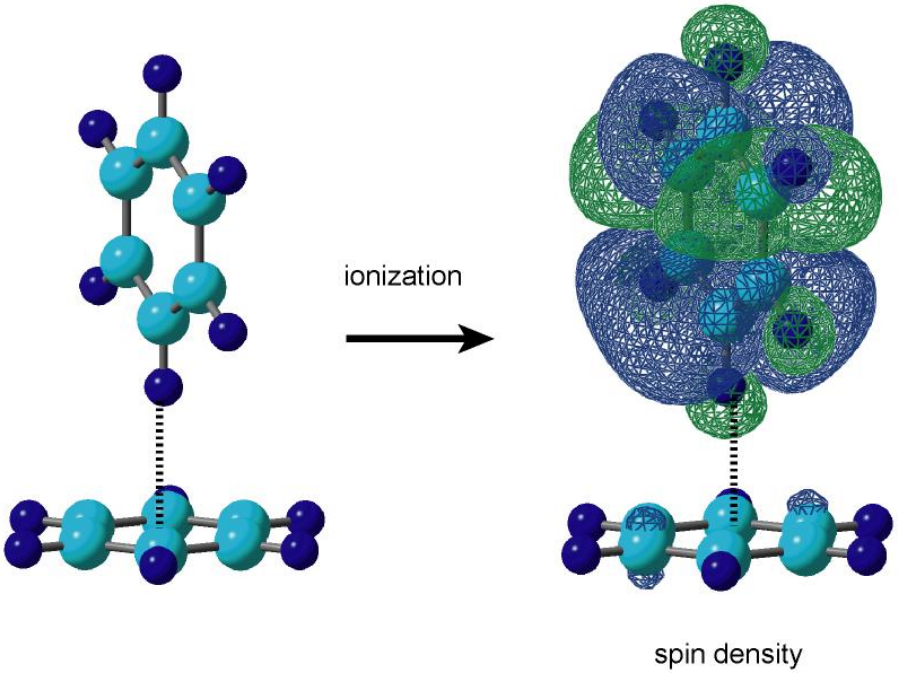

Figure S1. Spin density on the benzene dimer cation at vertical ionization point. The calculation was carried out at the MP2/6-31G(d) level of theory.

2. Effects of initial structures on the product channel.

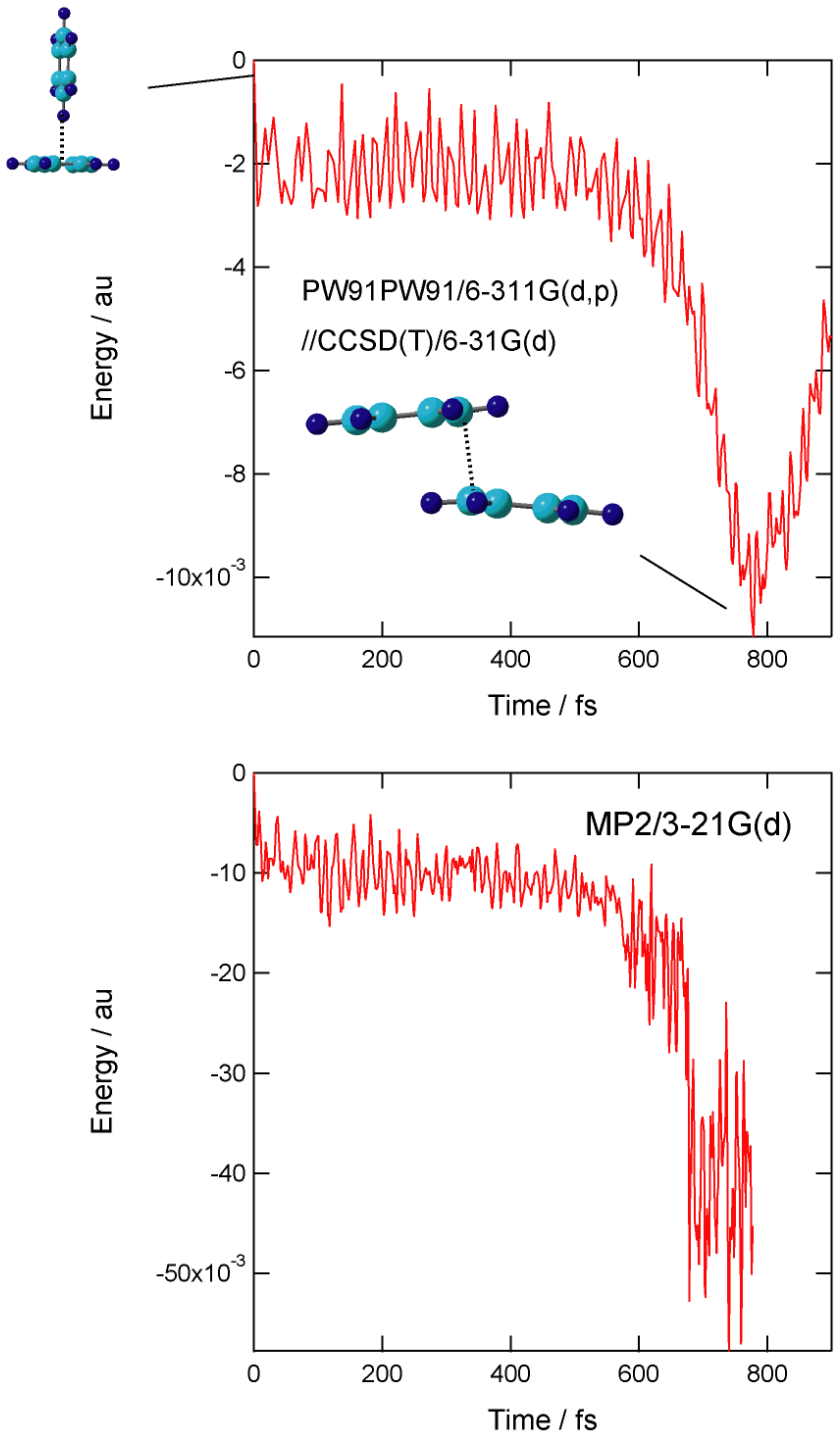

Figure S2. Time evolutions of potential energies of the ionization reaction of benzene dimer obtained by direct ab-initio MD calculation.