**Supplementary Material**

Equilibrium atomic conformation of Pt2Ru3 nanoparticles under gas atmosphere of CO/H2 investigated by density functional theory and Monte Carlo simulation

Md Khorshed Alama), and Hiromitsu Takabab)

Department of Environmental Chemistry and Chemical Engineering,

School of Advanced Engineering, Kogakuin University,

2665-1 Nakano, Hachioji, Tokyo 192-0015, Japan

a) Present address: Department of Physics, University of Barisal, Kornokathi, Barisal 8200, Bangladesh

b) Address all correspondence to this author. e-mail: [takaba@cc.kogakuin.ac.jp](mailto:takaba@cc.kogakuin.ac.jp)

FIG.S1

C:\Users\Khorshed\Desktop\Manuscript_2017\JMR-3\MRS Communication\Revised version\Final Revised version\FIG. S1.tif

**FIG.S1 Coadsorption models of CO with H2 on Pt2Ru3: (a) both CO and H2 coadsorb on Pt3Ru1/Pt1Ru3 (top two layers) H2 on Pt site CO on Ru site; (b) CO and H2 coadsorb on Pt3Ru1/Pt1Ru3 (top two layers) H2 on Ru site CO on Pt site; (c) CO and H2 coadsorb on Pt1Ru3/Pt2Ru2 (top two layers) H2 on Pt site CO on Ru site; (d) CO and H2 coadsorb on Pt1Ru3/Pt2Ru2 (top two layers) H2 on Ru site CO on Pt site;**