

## SUPPLEMENTARY INFORMATION

### **CH<sub>4</sub> dehydrogenation and H<sub>2</sub> formation on Pt (100) surface: an insight from the reactive molecular dynamics simulations**

Rizal Arifin<sup>1\*</sup>, Darminto<sup>2</sup>

1. Department of Mechanical Engineering, Universitas Muhammadiyah Ponorogo, Jl. Budi Utomo No. 10, Ponorogo, 63471, Indonesia
2. Department of Physics, Institut Teknologi Sepuluh Nopember, Kampus ITS Sukolilo, Surabaya, 60111, Indonesia

\*Corresponding author:

Dr. Rizal Arifin

e-mail: [rarifin@umpo.ac.id](mailto:rarifin@umpo.ac.id)

### SUPPLEMENTARY INFORMATION S1 and S2.

Supplementary information S1 and S2 are visualizations of CH<sub>4</sub> dissociation on the Pt (100) surface on the upper and lower surfaces, respectively. The files are in the format of MP4 and are uploaded to the Figshare repository in the following link: <https://doi.org/10.6084/m9.figshare.22718077>.

### SUPPLEMENTARY INFORMATION S3.

**Figure caption:** Initial (top) and final (bottom) radial distribution functions  $g(r)$  of the atomic pairs in the simulation system.



