Supplemental Information for “Reaction Mechanisms and Interfacial Behaviors of Sodium Silicate Glass in Aqueous Environment from Reactive Force Field Based Molecular Dynamics Simulations”

Lu Deng¹, Katsuaki Miyatani², Shin-ichi Amma³, Michinori Suehara², Madoka Ono³, Yuichi Yamamoto², Shingo Urata², and Jincheng Du¹,*

¹Department of Materials Science and Engineering, University of North Texas, Denton, Texas, U.S.A.
²Innovative Technology Laboratories, AGC Inc., Yokohama-shi, Kanagawa 221-8755, Japan
³Materials Integration Laboratories, AGC Inc., Yokohama-shi, Kanagawa 221-8755, Japan

(*Corresponding author. Email: du@unt.edu; Phone: 940-369-8184)

The averaged charge distributions along z direction (perpendicular to the glass-water interface) for 900K simulations at different simulation times are shown in Fig. S1.

Fig. S1 Charge distribution along Z direction of the configurations at different simulation time