Contact Charging between Insulators: A Theoretical Study

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***Abstract*— The mechanism of charging that occurs when a pair of insulating surfaces is rubbed remains poorly understood. It is not yet known which species are transferred during the charging process. To identify the charge species, atomic molecular level simulations of contact between particular crystallographic surfaces of single-crystal quartz (SiO_2) and Sapphire (Al_2O_3) are carried out in this study. This study was performed by SIESTA package. Both dry and saturated cases were investigated to confirm the charge transfer mechanism. For dry situation, results show that sapphire charged positively and quartz charged negatively. The correlation between this phenomena and has been established with electrostatic potential energy on both surfaces. This correlation has also been tested on another single crystal system, Periclase (MgO). Another focus is on observing ion transfer during the molecular dynamics trajectory by adding water into the system. Dissociation and interaction of water has been observed and hydroxyl ions (OH-) are likely to adsorb on Sapphire site and hydrogen ions (H+) on Quartz. Additional simulations were performed to quantitatively determine the parameters affecting ion transfer during the contact charging.**