Contact Charging between Surfaces of Quartz (0001) and Sapphire (0001) - 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. Mulliken population analysis was carried out to investigate the electron transfer mechanism. Results of this simulation show that Sapphire charged positively and quartz charged negatively. This phenomenon of charging has been observed in laboratory experiments on triboelectric charging in insulator systems. Another focus is on observing ion transfer during the molecular dynamics trajectory by adding water into the system. Additional simulations were performed to quantitatively determine the parameters affecting ion transfer during the contact charging.**