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Adsorption Characteristics of Binary Mixtures of Two Halomethanes on Graphite Surface[1] KIRAN KHANAL, Department of Polymer Science, The University of Akron, Akron, Ohio, GARY LEUTY, Air Force Research Lab, Dayton, Ohio, MESFIN TSIGE, Department of Polymer Science, The University of Akron, Akron, Ohio — Understanding the physisorption mechanism of mixtures of small molecules on graphite substrate has been a growing interest in materials science in order to investigate the changes in adsorption behavior of mixtures near interfaces vs. the individual components. Using atomic-scale molecular dynamics simulations, we have studied the structure and dynamics of multilayer adsorption of binary mixtures of two halomethanes (CF4 and CF3Cl) on graphite substrates for different bulk compositions of CF4. Simulations were performed in the temperature range 60-120K. The goal of this study is to explore how the compositions of individual components as well as temperature, affect the structure of films near the interface, the mobility of molecules, the molecular orientation and the substrate affinity. Preliminary results suggest a strong influence of the concentration of CF4 and temperature on the structure and mobility of molecules in first adsorbed layer on the graphite surface. In agreement with the recent experimental results, CF4 displaces CF3Cl from the first absorbed layer at all temperatures in our range and becomes the leading component in the mixture at high temperature for large CF4 concentrations in the mixture.

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