

Surface Coverages of Bonded-Phase Ligands on Silica: A Computational Study

Nikolay D. Zhuravlev and J. Ilja Siepmann

*Departments of Chemistry and of Chemical Engineering and Materials Science,
University of Minnesota, 207 Pleasant St. SE, Minneapolis, MN 55455*

Mark R. Schure

*Theoretical Separation Science Laboratory, Rohm & Haas Company,
727 Norristown Road, Springhouse, PA 19477*

Keywords: Reversed-phase Liquid Chromatography, Octadecylsilane (C₁₈) Phase, Silica Surfaces

Abstract

A computational study of the packing of various bonded-phase ligands bound to chromatographic silica is presented. This is done with the intention of examining the type of surface structures that are typically found in real chromatographic systems. Utilizing the surface structure of the (111) face of the β -cristobalite crystal it is shown that the maximum surface coverages of dimethyl octyl silane, dimethyl octadecyl silane, triisopropyl silane, diisopropyl octyl silane, and diisopropyl octadecyl silane can be calculated that are in good agreement with experiment. The maximum surface coverages are also calculated for the (100) face of the β -cristobalite crystal and for a set of random silica surfaces. The coverages for the latter two surface types are found to be significantly lower than the experimental values for chromatographic silica surfaces. These results further suggest that chromatographic silica surfaces may resemble crystalline surface sites similar to the (111) face of β -cristobalite, as has been previously suggested in the literature. Hence, these structures can be reliably utilized in molecular simulations of bonded-phase chromatography where the atomic-level detail of the silica surface has been previously lacking.