Introduction

Field-Effect Transistors (FETs) are becoming increasingly important due to their application in chemical and biomolecular sensing (e.g. Bio-FET sensors). FETs can easily be integrated into portable devices and can provide low-cost, real-time, label-free detection. Analyte is detected when it induces changes in the surface potential resulting in a measurable change in the current. Rational design of FET biosensors is currently hindered by a lack of models capable of accurate prediction of device response due to addition of biomolecular analyte, or due to changes in surface chemistry. Presently, response models are generally incapable of describing steric-effects due to the surface structure, the finite-size of molecules, or polarisation effects due to water or biomolecule orientation. To address this limitation, explicit solvent Molecular Dynamics simulations were performed of the silicon dioxide-electrolyte interface.

Simulation and Results

In these simulations, the surface charge was varied and the surface potential calculated in order to generate an effective pH/surface potential response curve. This simulated potential, shown in Figure 1, shows agreement with experimental potentiometric data for low surface charge densities (less than approximately pH 9), supporting the validity of this approach as a novel technique of predicting FET-sensor response. This simulation technique can be used as a tool for improving our understanding of the mechanism of response of potentiometric sensors such as FET-sensors, and therefore rational improvement of biosensor response.

Figure 1 – Electrostatic surface potential as a function of surface charge density, simulated by molecular dynamics simulation of the silica-electrolyte interface (300 mM NaCl, explicit solvent)