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Ab initio molecular dynamics study of the electric double-layer capacitance at solution-electrode interfaces YASUNOBU ANDO, YOSHIHIRO GOHDA, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo — Electric double-layer (EDL) is known as an important stage for electrochemical reactions at electrode-liquid interfaces. It has also attracted growing interest for its applications to electronic devices, called EDL capacitors (supercapacitors) and EDL transistors. In efficient development of each device, predicting the EDL capacitance in light of the material features is required. However, Helmholtz capacitance, the part of the EDL capacitance depending on the microscopic structure, has still not been estimated theoretically. Therefore, to evaluate that, we calculated the structure of solution-electrode interfaces by using ab initio molecular dynamics with effective screening medium method. As a result, we made it possible to estimate the Helmholtz capacitance taking the effect of the molecular orientation of the water and the electronic polarization in the water molecules due to the electric field into account. Apparent dielectric constant of the water near the interface can also be calculated. Interestingly, the results reveal that the existence of a first layer of the water molecules near the electrode determines the distance of closest approach of hydrated ions. Moreover, the estimated dielectric constant of the first layer differs from that predicted by the classical theory.

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