「Multicanonical algorithm in Ab initio simulation: investigation of structure and spectroscopy of clusters.」

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講演タイトル	「Multicanonical algorithm in Ab initio simulation: investigation of structure and spectroscopy of clusters.」
講演概略	The talk will start with an introduction of multicanonical and histogram reweighting techniques. Later how ab initio Monte Carlo simulation with multicanonical algorithm can investigate properties of clusters at various temperature will be discussed. Two examples will be preseneted. The first one is the average structural change of water dimer as a function of temperature. In this work average structure of water dimer was monitored as a function of temperature by means of several radial and angular distribution functions. In the second example, highly complex photoelectron spectra of Si2C2- will be assigned from the first principle. The complexity of the spectra is due to two isomers at the experimental condition. The broad peaks in the spectra come from the floppy isomer. Multicanonical/reweighting technique is found to be a robust technique for elucidating finite temperature effects on molecular systems.