



演題：**Global-switching trajectory surface-hopping  
algorithm for conical intersections and  
intersystem crossings with its application to  
photochemistry**

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本講演は、総合化学院「化学研究先端講義(修士課程選択科目)/総合化学特別研究第二(博士後期課程選択科目)」の授業の一環として開催します。

要旨：

We have developed global-switching trajectory surface-hopping algorithm to treat both conical intersections and intersystem crossings on an equal footing for nonadiabatic photophysical and photochemical processes. For the conical intersections, we simulate switching probability estimated from electronically adiabatic potential energy surfaces and its gradients along on-the-fly trajectory. For the intersystem crossings, we simulate switching probability estimated from constant spin-orbital couplings. In this way, the present global-switching algorithm is computationally much faster than Tully's fewest-switching algorithm. Several prototypical examples of photoisomerization and photochemical reaction involving multi-state nonadiabatic transitions are addressed in comparison with experimental results.

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