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Correction to "SHARC — *Ab Initio* Molecular Dynamics with Surface Hopping in the Adiabatic Representation Including Arbitrary Couplings" [*J. Chem. Theory Comput.* 2011, *7*, 1253−1258]

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In a recent paper,[1] we lined out a novel *ab initio* molecular dynamics (MD) method termed SHARC, which is able to treat arbitrary couplings in molecular systems including all degrees of freedom. The basis is Tully's surface hopping scheme,[2] as it is for several other methods, see e.g. refs 3−8. Laser-induced couplings were treated in the surface hopping formalism for the first time by Thachuk et al.[3] and later on by Jones et al.[5] as well as Mitrić et al.[6] However, to our knowledge, we have treated spin−orbit coupling and dipole couplings simultaneously for the first time in MD. In a first test case, we validated the ability of our new method to describe laser coupling only. To this aim, we used two displaced harmonic oscillators. The same model was employed before by Mitrić and co-workers using the so-called FISH method in ref 36 of our paper (here ref 6); the latter methodology is shown to be a very good approximation to interpret some laser control experiments.[9−12] Unfortunately, we did not point out clearly in ref 1 that the parameters of the test system were taken from the aforementioned source, which we hereby do. In ref 1, we repeated the simulations on the model system and obtained the same results as Mitrić and co-workers, in agreement with exact quantum dynamics. This means that the FISH and SHARC methods yield identical results for this case. Yet, there may be significant differences in the performance of the SHARC method compared to the FISH method for certain problems. Both methods, although technically different, serve to pursue the same goal, namely, to unravel unknown photochemical processes and mechanisms in large molecules including all degrees of freedom.

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