Global analytical potential energy surfaces: Searching for symmetry adapted functional forms

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In this review, the derivation of analytical, full-dimensional and global representations of potential energy surfaces in the lowest adiabatic electronic state of a generic XY_n type of molecule is discussed. One focus is the general strategy to be adopted such that both spectroscopically relevant features of the PES representation in the lower energy regions as well as kinetically relevant reaction channels in the higher energy regions are equally well treated. A second important aspect is the mathematically challenging derivation of adequate symmetry adapted functional forms to be used in the analytical representation. Concepts and theory will be illustrated at the examples of recent developments for the derivation of PES representations in "rigid" molecules such as methane [1, 2] as well as in "floppy" molecules such as ammonia [3, 4].

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[3] R. Marquardt, K. Sagui, W. Klopper, and M. Quack, J. Phys. Chem. B, **109**, 8439–8451 (2005).

[4] R. Marquardt, K. Sagui, J. Zheng, W. Thiel, S. Yurchenko, D. Luckhaus, F. Mariotti, and M. Quack. Work in progress.