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Stachó, László L.; Dömötör, Gyula; Bán, Miklós I.

Misgivings from the theoretical foundation of the path-following procedures based on the Elber–Karplus strategy. (English)

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Summary: A mathematical proof against the theoretical foundation of the Elber–Karplus (EK) global reaction path-following method and the improvements based on the EK strategy have been discussed. According to our arguments the minimization of the average value of the potential energy along a path to two energy minima never defines a reaction path (RP) unless in the chemically unrealistic situation where the points of the curve joining the two minima of reactants and products have constant energy values. Therefore, finding approximate RPs by EK-strategies for large chemical systems or even in mathematical test examples is impossible or at least strongly doubtful (the larger the system the more doubtful).

Classification :

***92E20** Chemical flows, reactions, etc.