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BOOK OF ABSTRACTS

Comparative Study of Global Path-Following Methods

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Global path-following algorithms[1-4] based on the strategy of the Elber-Karplus method[5], especially those coupled with molecular mechanics, are quite popular and widely used for the calculations of potential energy surfaces of large organic- and biomolecules. Another type of this sort is the DDRP method[6]. To have a comparison about the stability, computation time, accuracy, etc. of the different methods, calculations were per- formed on some mathematical test-functions (e.g. the curves of Müller-Brown[7] and Stachó-Bán[6,8]). The results of calculations prove our preliminary expectations, i.e. the superiority of the stability of the DDRP method over other algorithms.

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