

Alanine diPeptide

The Alanine DiPeptide (DA) is one of the basic objects for studies of molecular dynamics. We have animated a 'DA dance' that includes the 9 low energy positions of DA as calculated via MD simulations by Wang and Duan (J. Com. Chem., 2004). The path of the animation was reported on the energy landscape (Fig.) and shows that high energy peaks (clear areas in the map) are avoided.

The low energy positions are marked by a flash light in the animation, and by white circles in the energy map.

