Contribution ID: **6** Type: **Oral Presentation**

Concavity of energy surfaces

Wednesday, 10 July 2013 10:50 (20 minutes)

Abstract content
   (Max 300 words)

The property of concavity in calculations of energy surfaces is developed and discussed, in reference to strict energy minimization when collective coordinates are constrained. Such collective coordinates are actually subject to quantum fluctuations and these prevent, via tunnel effects, the probing of maxima and saddle points. A solution to the problem is developed. It allows to bypass the concavity syndrome and recover maxima and saddle points.

Apply to be
 considered for a student
   award (Yes / No)?

No

Would you like to <br> submit a short paper <br> for the Conference
 Proceedings (Yes / No)?

Yes

Primary author: Prof. KARATAGLIDIS, Steven (University of Johannesburg)

Co-author: Prof. GIRAUD, Bertrand (CEA/Saclay)

Presenter: Prof. KARATAGLIDIS, Steven (University of Johannesburg)

Session Classification: Theoretical

Track Classification: Track G - Theoretical and Computational Physics