Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information (ESI) for "*Ab Initio* Conical Intersections for the Si(^{1}D)+H_2 Reaction System: A Lowest Five Singlet States Study"

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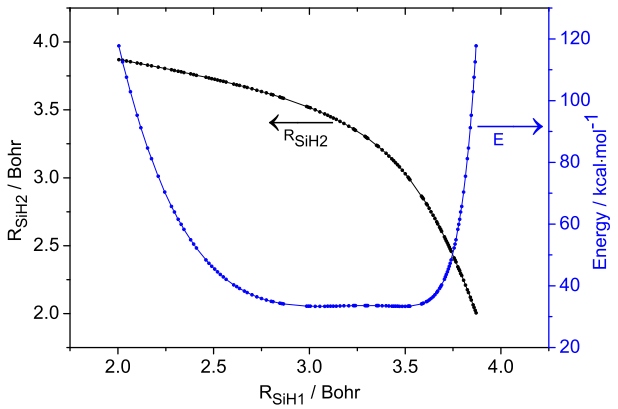
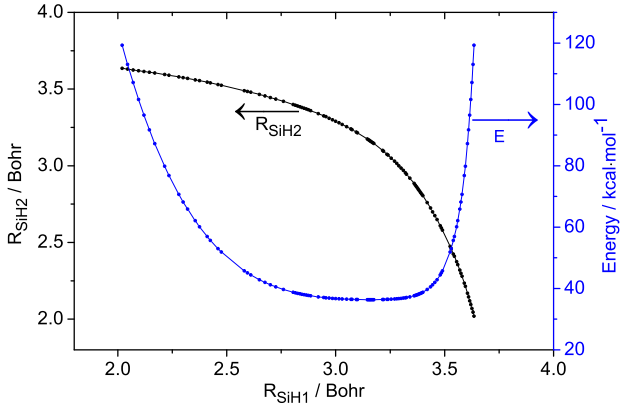
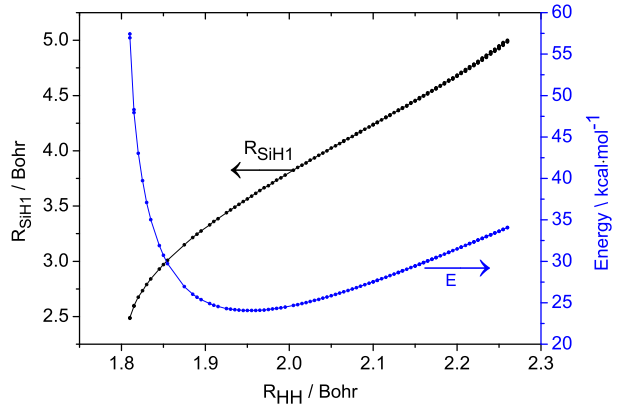


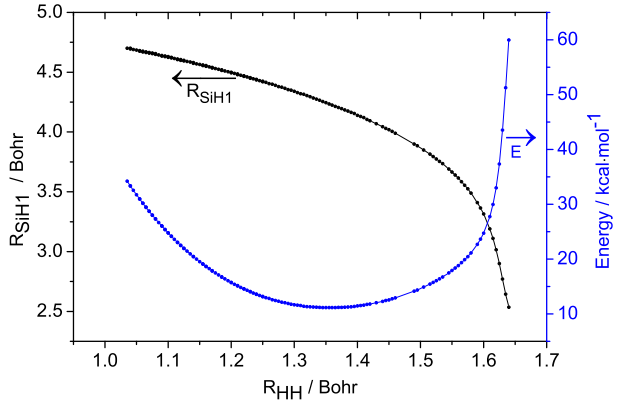
(a) The $1^1A'(1^1A'')$–$2^1A'(2^1A'')$ intersection at linear H-Si-H geometries.



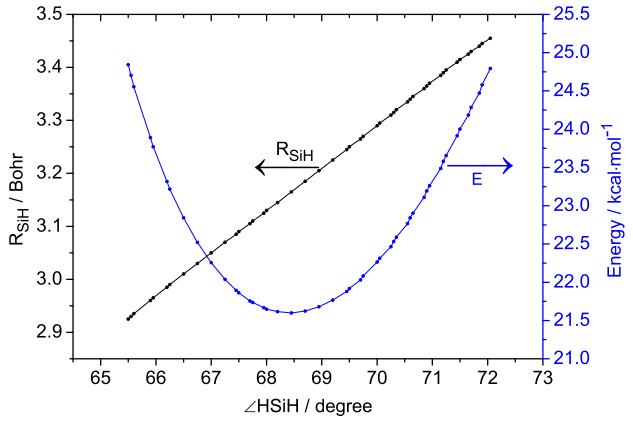
(b) The $2^1A'(2^1A'')$–$3^1A'(2^1A'')$ intersection at linear H-Si-H geometries.



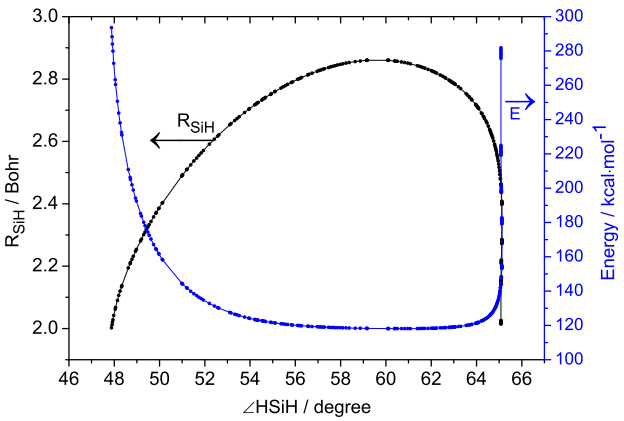
(c) The $1^1A'(1^1A'')$–$2^1A'(2^1A'')$ intersection at linear Si-H-H geometries.



(d) The $2^1A'(2^1A'')$–$3^1A'(2^1A'')$ intersection at linear Si-H-H geometries.

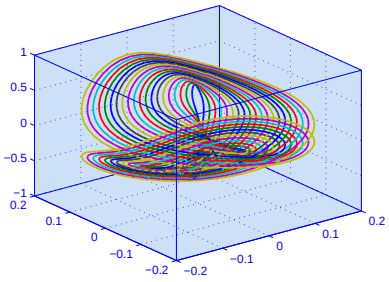


(e) The $1^1A''$–$2^1A''$ intersection at C_{2v} geometries.

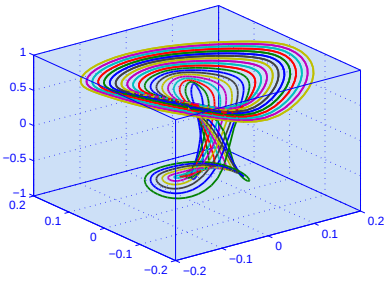


(f) The $2^1A'$–$3^1A'$ intersection at C_{2v} geometries.

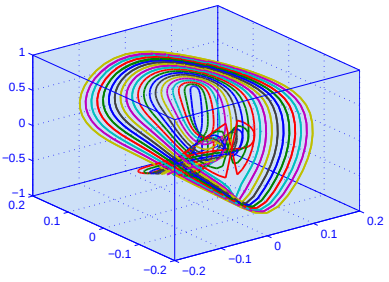
Fig S1. The seam lines of the intersection at linear H-Si-H geometries(a,b), linear Si-H-H geometries(c,d) and C_{2v} geometries(e,f). The energies are relative to Si(^{1}D)+H_2 asymptote.



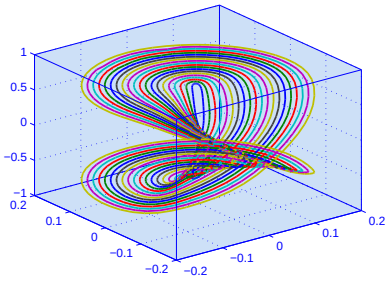
(g) $1^1A'$ state in $1^1A'(1^1A'')$–$2^1A'(2^1A'')$ intersection at linear H-Si-H geometries.



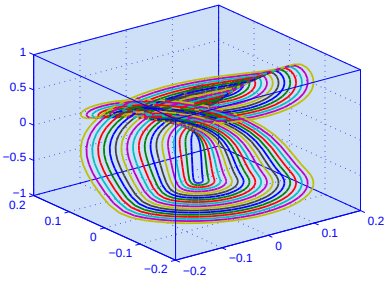
(h) $2^1A'$ state in $1^1A'(1^1A'')$–$2^1A'(2^1A'')$ intersection at linear H-Si-H geometries.



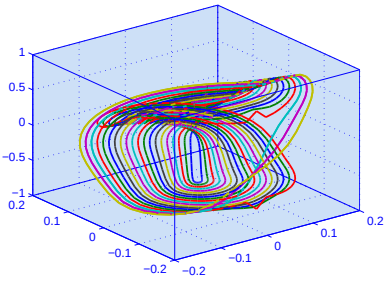
(i) $2^1A'$ state in $2^1A'(2^1A'')$–$3^1A'(2^1A'')$ intersection at linear H-Si-H geometries.



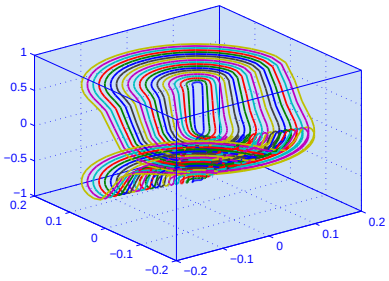
(j) $3^1A'$ state in $2^1A'(2^1A'')$–$3^1A'(2^1A'')$ intersection at linear H-Si-H geometries.



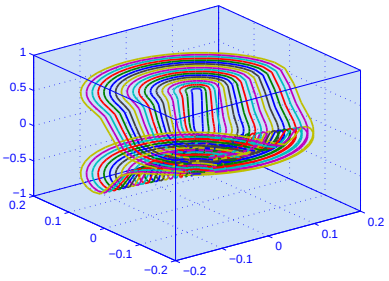
(k) $1^1A'$ state in $1^1A'(1^1A'')$–$2^1A'(2^1A'')$ intersection at linear Si-H-H geometries.



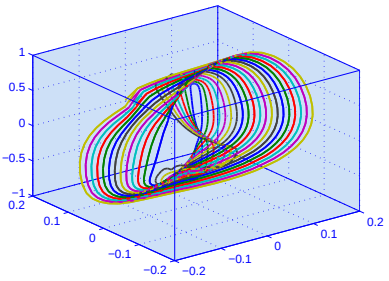
(l) $2^1A'$ state in $1^1A'(1^1A'')$–$2^1A'(2^1A'')$ intersection at linear Si-H-H geometries.



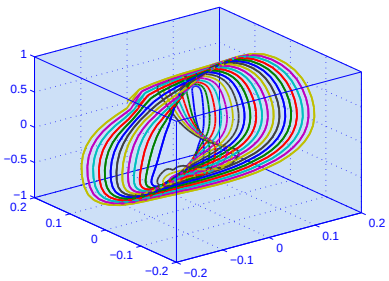
(m) $2^1A'$ state in $2^1A'(2^1A'')$–$3^1A'(2^1A'')$ intersection at linear Si-H-H geometries.



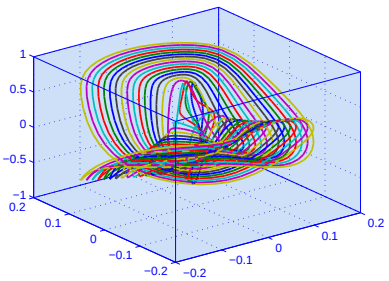
(n) $3^1A'$ state in $2^1A'(2^1A'')$–$3^1A'(2^1A'')$ intersection at linear Si-H-H geometries.



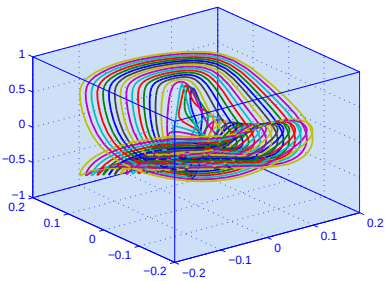
(o) $1^1A''$ state in $1^1A''$–$2^1A''$ intersection at C_{2v} geometries.



(p) $2^1A''$ state in $1^1A''$–$2^1A''$ intersection at C_{2v} geometries.



(q) $2^1A'$ state in $2^1A'$–$3^1A'$ intersection at C_{2v} geometries.



(r) $3^1A'$ state in $2^1A'$–$3^1A'$ intersection at C_{2v} geometries.

Fig S2. The geometric phase effects associated with the conical intersections in Si(^{1}D)+H_2 system.