Electron scattering by Silane

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Introduction

Silane is an important molecule with numerous applications to natural & technological plasmas. In such environments, electron induced reactions plays a major role in its chemistry. In view of this, electron induced scattering of silane finds significance. The present article reports a comprehensive study of electron impact cross section (cs) for silane. In particular, the emphasis is given in providing a complete dataset for various e-scattering events possible with silane. Such data are needed to plasma modeling community. Moreover, the cs data are essential input to technological and fusion edge plasmas and in dynamic plasma models to study the particle interactions & the properties of the plasma [1]. The total cross sections for electron scattering from gaseous molecules are also necessary to high resolution plasma processing, simulating the glow discharge & in semiconductor industry .

Theoretical methodology

The theoretical methods employed here comprises of two formalisms namely R-matrix and the SCOP. The inner region wave function in R-matrix method is given by,

$$\psi_k^{N+1} = A\sum_I \psi_I^N(x_1,\cdots,x_N)\sum_j \xi_j(x_{N+1})a_{Ijk} + \sum_m \chi_m(x_1,\cdots,x_{N+1})b_{mk}$$

In Spherical Complex Optical Potential (SCOP) formalism, The potential employed here is spherical and complex and hence the name Spherical Complex Optical Potential formalism, which is given by,

$$V(r,E_i) = V_{st}(r) + V_{ex}(r,E_i) + V_{pol}(r,E_i) + iV_{abs}(r,E_i)$$

The Schrodinger equation is then solved using the potential through partial wave analysis, which gives phase shifts. Employing the phase shifts cross sections values are derived.

Target Properties

Properties of SiH4	Present DZP	Experimental	Theoretical
Ground-state energy (hartrees)	-291.252089	-	-291.359885 [11]
First excitation energy (eV)	9.8554	8.7 [12]	9.88 [13]
Rotational constant (cm^{-1})	2.864	2.865 [11]	
Dipole moment (au)	0	0 [11]	

Results

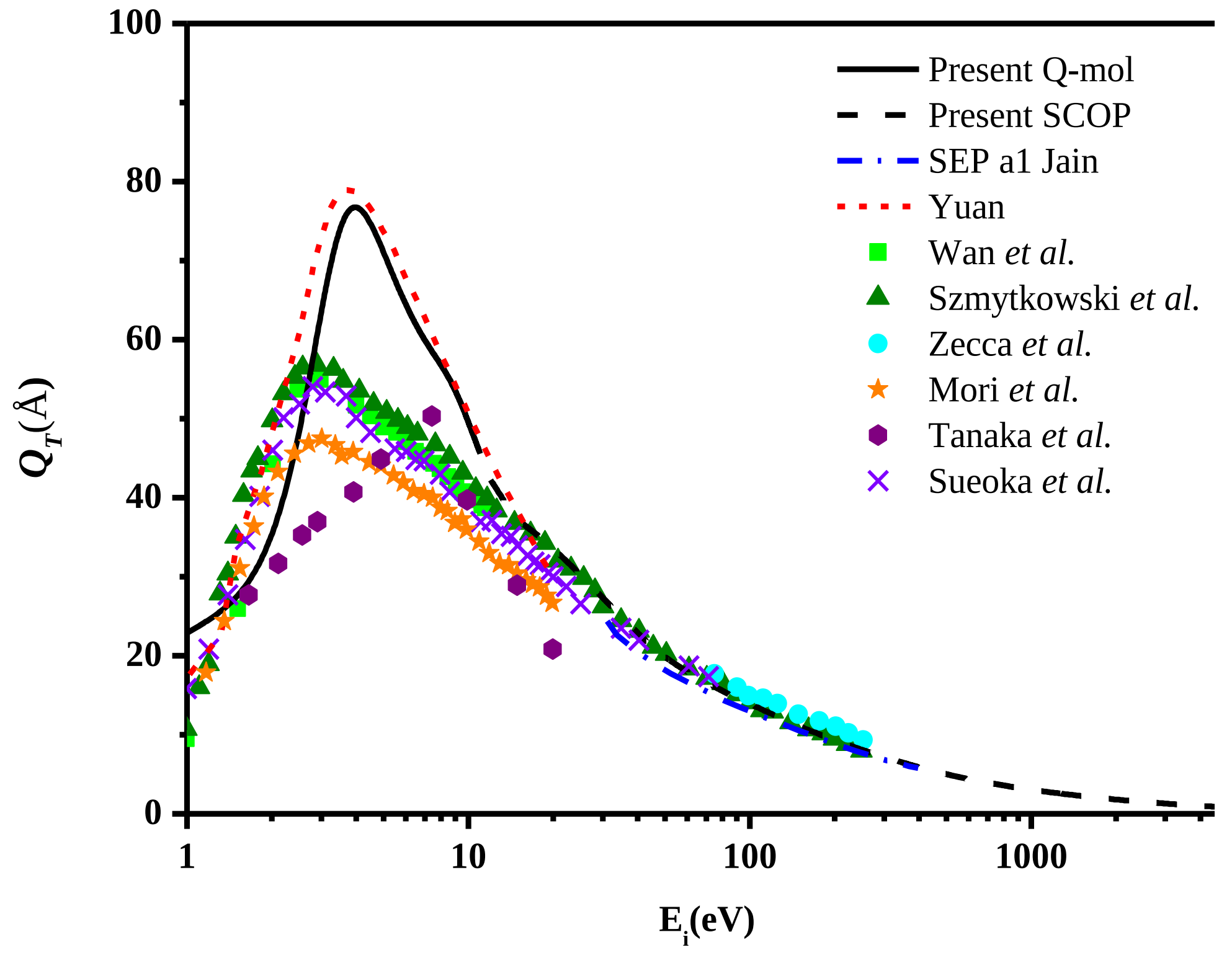


Fig 1 *:* Total cross section

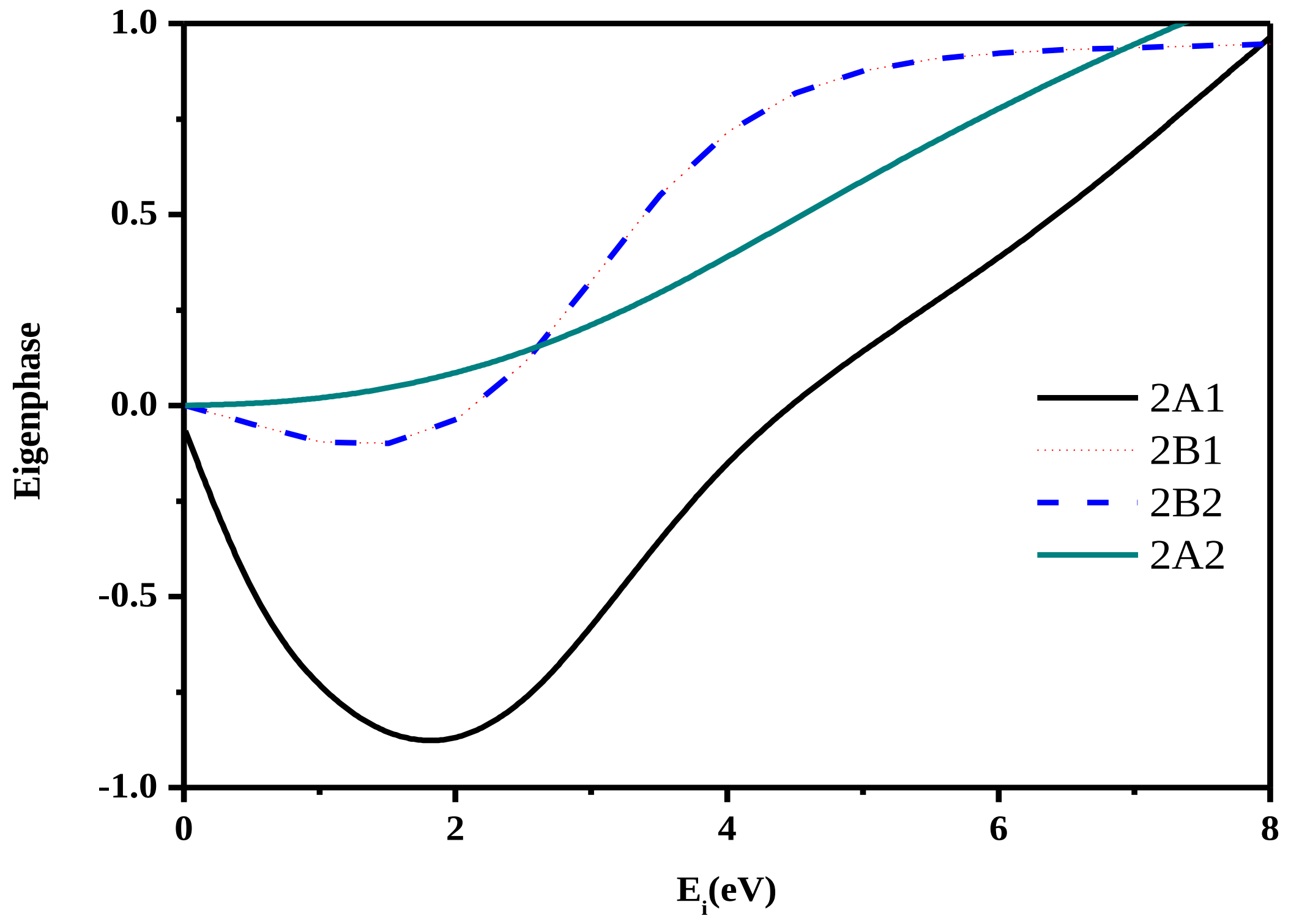
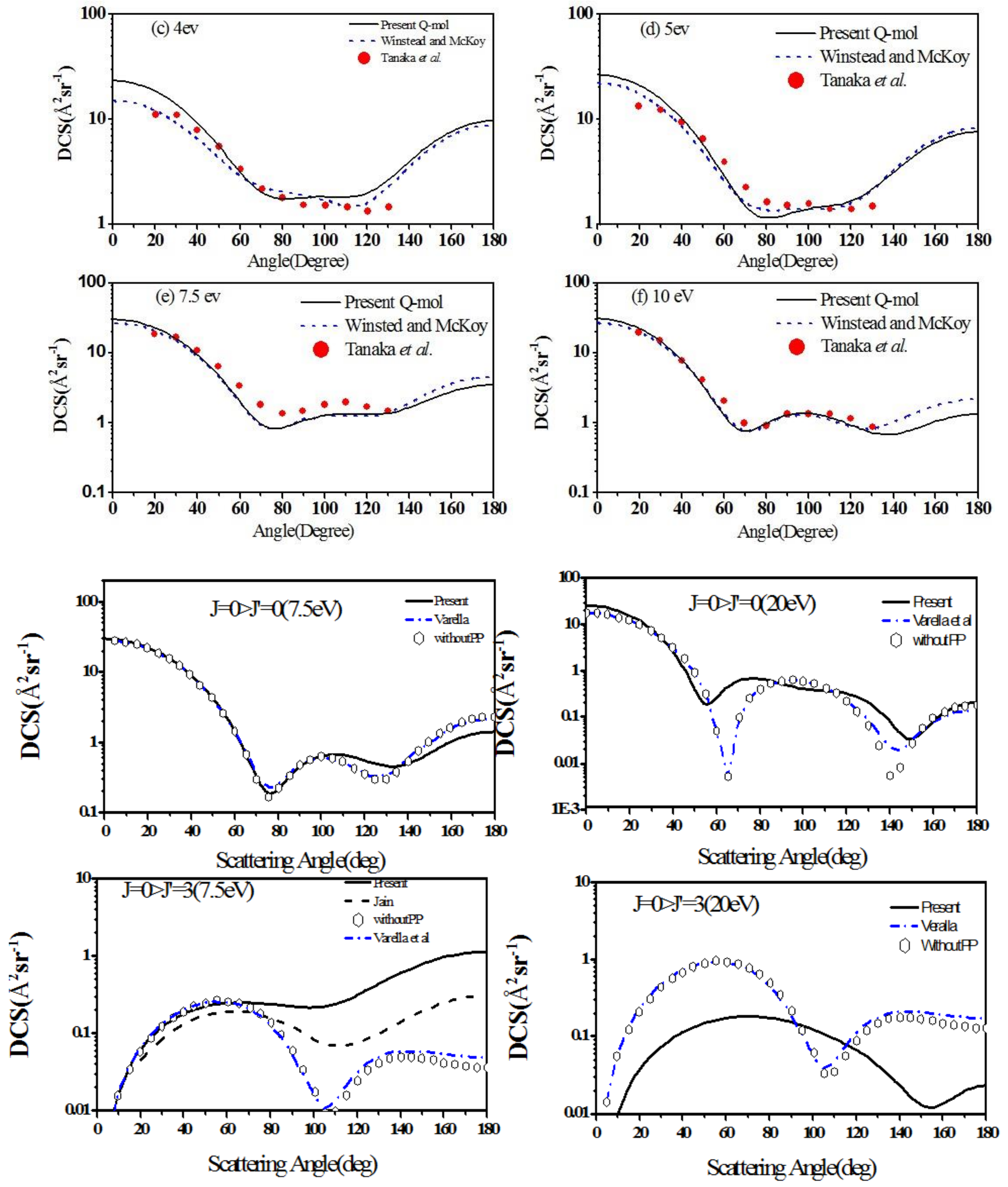


Fig:3 Eigen phase sum



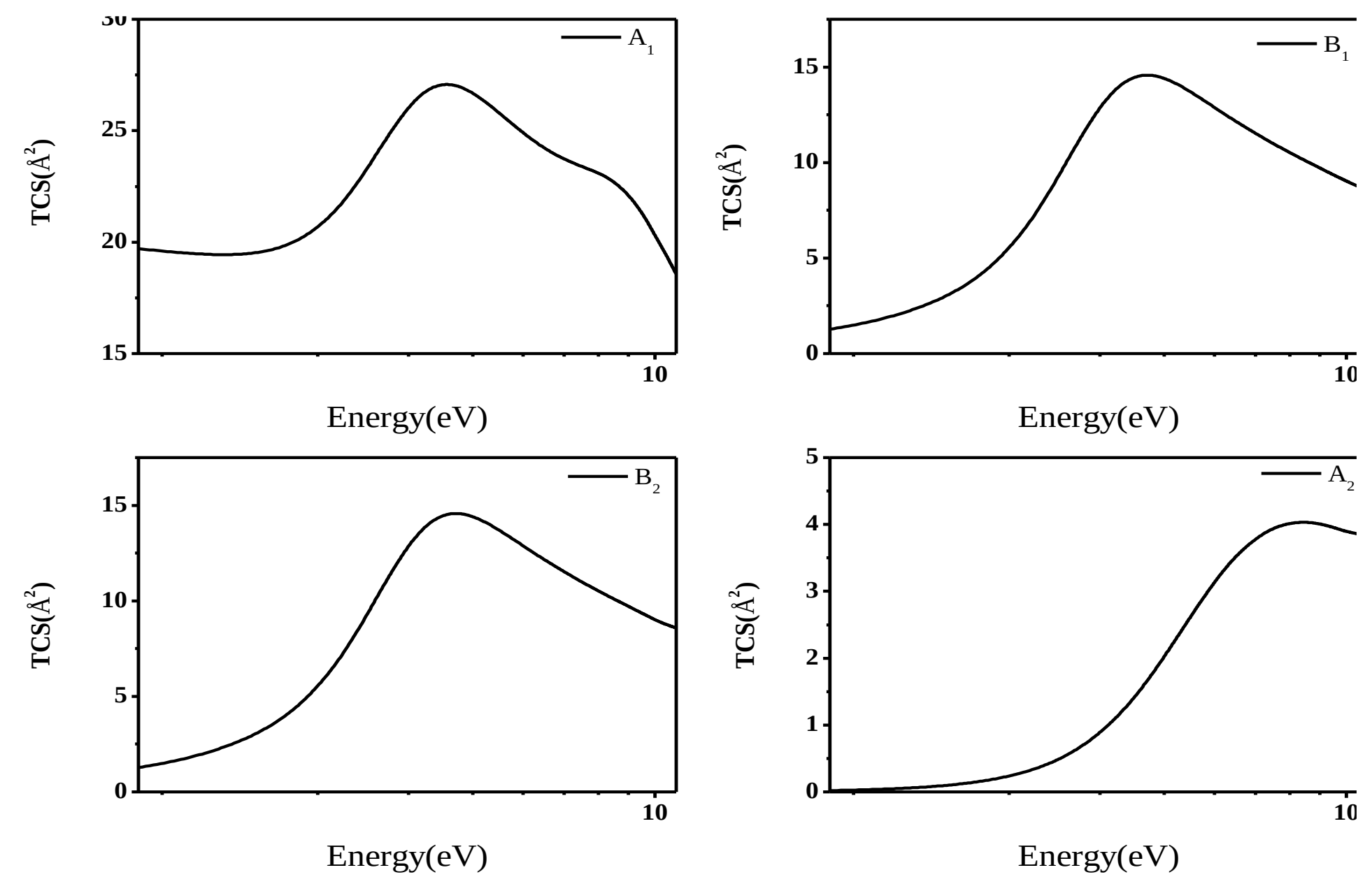


Fig 2 : Symmetry component of TCS

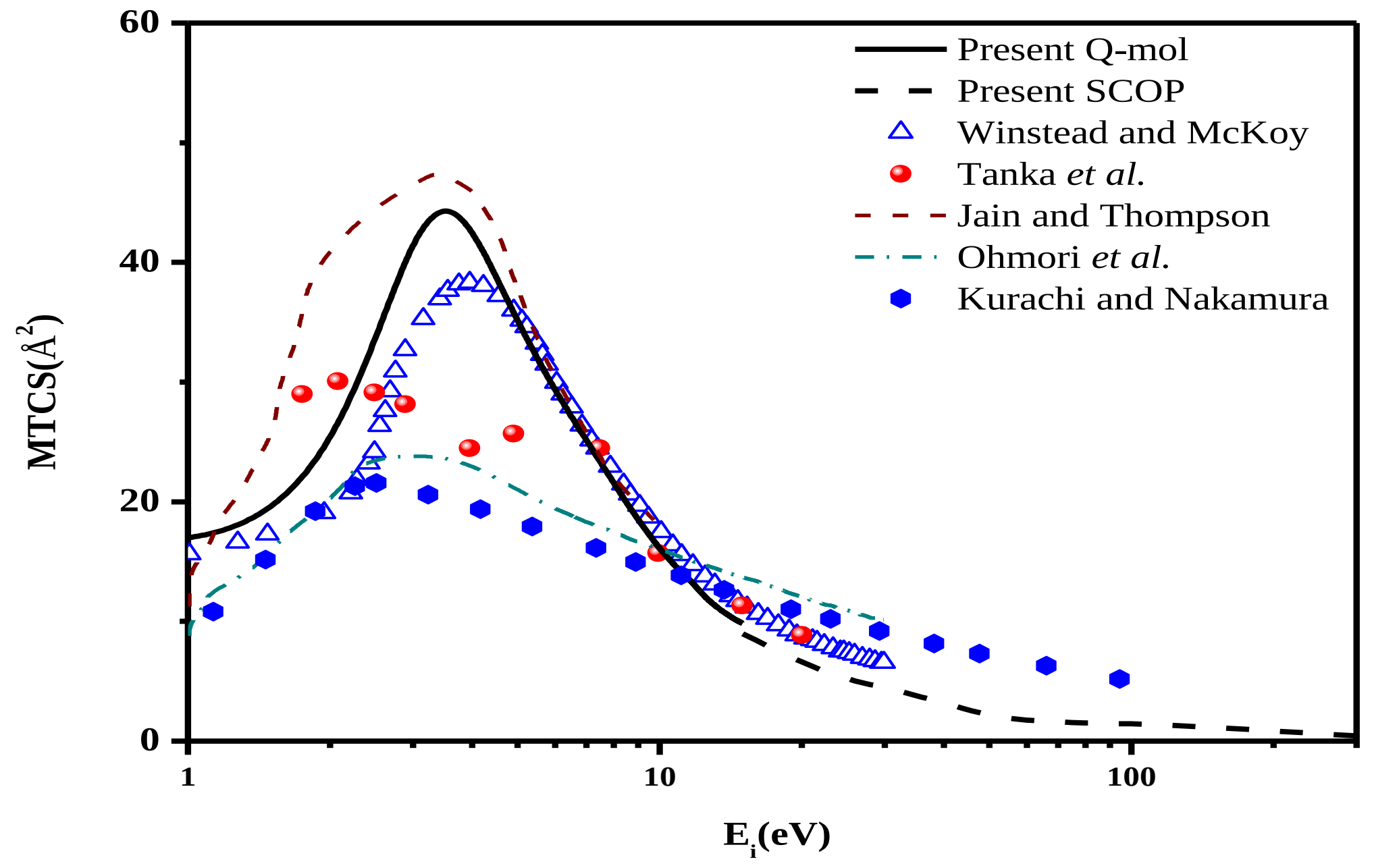


Fig4: MTCS

Fig 5 :Elastic DCS and DCS for rotational excitation

Conclusion

- ➢The methodologies employed here are the R-matrix method for low energy regime and the SCOP formalism for intermediate to 5000 eV.
- ➢The TCS obtained agrees well in terms of nature and shape of the curve with all the available experimental and theoretical values.
- ➢A shape resonance is detected around 3.35 eV due to degenerate B_1 and B_2 symmetries.
- ➢The present DCS shows good agreement with the experimental and theoretical data of Tanaka *et al*.[12] and Winstead and Mckoy [6].
- ➢The formation of various anionic fragments (SiH_3^-, SiH_2^-, H^-, SiH^-, Si^-, H^-) [9-11] fragments occurs with total anion yield falling around 8.75 eV.
- ➢The consistency of the results obtained by the two formalisms is quite good and shows a smooth transition at the overlapping energy (at around 11eV).

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