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The VOLSCAT package for electron and positron scattering of molecular targets: A new high throughput approach to cross-section and resonances computation. (English)

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Summary: `VOLSCAT` is a computer program which implements the Single Center Expansion (SCE) method to solve the scattering equation for the elastic collision of electrons/positrons off molecular targets. The scattering potential needed is calculated by on-the-fly calls to the external SCELib library for molecular properties, recently ported to GPU computing environment and ClearSpeed platforms, and made available by means of an Application Program Interface (SCELib-API) which is also provided with the VOLSCAT package in a *beta* version. The result is a high throughput approach to the solution of the complex e^-/e^+-molecule scattering problem, with allows for intensive calculations both for the number of systems which can be studied and for their size. Accurate partial and total elastic cross sections are produced in output together with the associated eigenphase sums. Indirect scattering processes arising from the formation of temporary negative ions can also be analyzed through the computation of the resonances' parameters.

MSC:

81-04 Software, source code, etc. for problems pertaining to quantum theory

Keywords:

single center expansion library; SCE molecular properties; electron-molecule scattering; `VOLSCAT`

Software:

GAUSSIAN; SCELib; VOLSCAT

Full Text: DOI

References:

[1] von Sonntag, C., The chemical basis of radiation biology, (1987), Taylor and Francis London
[2] Simons, J., Acc. chem. res., 39, 772, (2006)
[3] Baccarelli, I.; Gianturco, F.A.; Grandi, A.; Lucchese, R.R.; Sanna, N., Adv. quantum chem., 52, 189, (2007)
[4] Sanche, L., Eur. phys. J. D, 35, 367, (2005)
[5] Boudaiffa, B.; Cloutier, P.; Hunting, D.; Huels, M.A.; Sanche, L., Science, 287, 1658, (2000)
[6] Gianturco, F.A.; Thompson, D.G.; Jain, A., Computational methods for electron – molecule collisions, (1995), Plenum New York
[7] Lucchese, R.R.; Gianturco, F.A., Int. rev. phys. chem., 15, 429, (1996)
[8] Altman, S.L.; Herzig, P., Point-group theory tables, (1994), Oxford University Press Oxford
[9] Frisch, M.J., Gaussian 03, revision C.02, 2004, (2004), Gaussian, Inc. Wallingford, CT
[10] Gianturco, F.; Rodriguez-Ruiz, J.A.; Sanna, N., Phys. rev. A, 52, 1257, (1995)
[11] Gianturco, F.A.; Jain, A.; Pantano, L.C., J. phys. B: at. mol. phys., 20, 571, (1987)
[12] Hara, S.J., J. phys. soc. jpn, 22, 710, (1967)
[13] Salvini, S.; Thompson, D.G., J. phys. B, 14, 3797, (1981)
[14] Gianturco, F.; Scialla, S., Electron – molecule scattering and photoionization, (1986), Plenum Publ. Co. New York
[15] Sham, L.; Kohn, V., Phys. rev., 145, 561, (1966)
[16] Gianturco, F.A.; Scialla, S., J. phys. B: at. mol. phys., 20, 3171, (1987)
[17] Gianturco, F.A.; Pantano, L.; Scialla, S., Phys. rev. A, 36, 557, (1987)
[18] Gianturco, F.A.; Sanna, N., Comput. phys. comm., 128, 139, (2000)
[19] Sanna, N.; Morelli, G., Comput. phys. comm., 162, 51, (2004)

[20] Sanna, N.; Baccarelli, I.; Morelli, G., Comput. phys. comm., 180, 12, 2544-2549, (2009), this issue

[21] Baccarelli, I., J. am. chem. soc., 129, 6269, (2007)

[22] Baccarelli, I.; Gianturco, F.A.; Grandi, A.; Sanna, N., Int. J. quant. chem., 108, 1878, (2008)

[23] Baccarelli, I.; Sanna, N.; Gianturco, F.A.; Sebastianelli, F., J. phys. conf. ser., 115, 012009, (2008)

[24] Gianturco, F.; Sebastianelli, F.; Lucchese, R.; Baccarelli, I.; Sanna, N., J. chem. phys., 128, 17430, (2008)

[25] Gianturco, F.; Lucchese, R., J. phys. chem. A, 108, 7056, (2004)

[26] Baccarelli, I.; Grandi, A.; Gianturco, F.A.; Lucchese, R.R.; Sanna, N., J. phys. chem. B, 110, 26240, (2006)

[27] Gianturco, F.; Lucchese, R., New J. phys., 6, 66, (2004)

[28] Gianturco, F., Eur. phys. J. D, 35, 417, (2005)

[29] Goumans, T.; Gianturco, F.; Sebastianelli, F.; Baccarelli, I.; Rivail, J.L., J. chem. theory comput., 5, 217, (2009)