Examples of Dedicated Software for performing (E)VB calculations

XMVB

(a) L. Song, Z. Chen F. Ying, J. Song, X. Chen, P. Su, Y. Mo, Q. Zhang, W. Wu, XMVB 2.0: An *ab initio* Non-Orthogonal Valence Bond Program, Xiamen University, Xiamen 361005, China, 2012. (b) L. Song, Y. Mo, Q. Zhang, W. Wu. *J. Comput. Chem.* 2005, **26**, 514. (c) Z. Chen, X. Chen, W. Wu, *J. Chem. Phys.* 2013, **138**, 164120.

Web site: http://xmvb.org
Integrated into GAMESS

VB2000

(a) J. Li, B. Duke, and R. McWeeny, VB2000 Version 2.0, SciNet Technologies, San Diego, CA, 2007. (b) J. Li, and R. McWeeny, VB2000: Pushing Valence Bond Theory to New Limits, *Int. J. Quantum Chem*., 2002, **89**, 208.

Web site: http://www.scinetec.com
Integrated into GAMESS

TURTLE

(a) J. H. van Lenthe, F. Dijkstra, W. A. Havenith, in Valence Bond Theory, D. L. Cooper, Ed., Elsivier, Amsterdam, The Netherlands, 2002, pp. 79-116, TURTLE - a gradient VBSCF Program Theory and Studies of Aromaticity. (b) J. Verbeek, J. H. Langenberg, C. P. Byrman, F. Dijkstra, J. H. van Lenthe, TURTLE: An ab-initio VB/VBSCF Program (1998-2000).

Integrated into GAMESS-UK

CRUNCH

(a) G. A. Gallup, R. L. Vance, J. R. Collins, J. M. Norbeck, Practical Valnce Bond Calculations. *Adv. Quant. Chem.* 1982, **16**, 229. (b) G. A. Gallup, The CRUNCH Suite of Atomic and Molecular Structure Programs, 2001. ggallup@phy-ggallup.unl.edu

MOLARIS-XG

Web site: http://laetro.usc.edu/software.html

Q

J. Marelius, K. Kolmodin, I. Feierberg, J. Åqvist, Q : An MD Program for Free Energy Calculations and Empirical Valence Bond Simulations in Biomolecular Systems. *J. Mol. Graph. Model.* 2013, 16, 213.

Web site: http://xray.bmc.uu.se/~aqwww/q/

VB/MM

(a) A. Shurki, H. Crown "ab initio VB/MM - A Valence Bond Ride through Classical Landscapes" J Phys. Chem. B 2005, **109**, 23638 (b) A. Sharir-Ivry, T. Shnerb, M. Strajbl, A. Shurki, "VB/MM Protein Landscapes: ab initio VB/MM Study of the SN2 Reaction in Haloalkane Dehalogenase" J. Phys. Chem. B 2010, **114**, 2212.

The VB/MM combines the XMVB package and a slightly modified MOLARIS package via a script which can be obtained from:

avitalsh@ekmd.huji.ac.il

Also Implemented In:

AMBER

D.A. Case, V. Babin, J.T. Berryman, R.M. Betz, Q. Cai, D.S. Cerutti, T.E. Cheatham, III, T.A. Darden, R.E. Duke, H. Gohlke, A.W. Goetz, S. Gusarov, N. Homeyer, P. Janowski, J. Kaus, I. Kolossváry, A. Kovalenko, T.S. Lee, S. LeGrand, T. Luchko, R. Luo, B. Madej, K.M. Merz, F. Paesani, D.R. Roe, A. Roitberg, C. Sagui, R. Salomon-Ferrer, G. Seabra, C.L. Simmerling, W. Smith, J. Swails, R.C. Walker, J. Wang, R.M. Wolf, X. Wu and P.A. Kollman (2014), AMBER 14, University of California, San Francisco.

Web site: http://ambermd.org

Please note that this list is not comprehensive, however, it directs the reader to the most commonly used current software packages for performing (E)VB calculations. Additionally, that a simple online application for performing EVB calculations made by Miha Purg at Uppsala University can be found at: http://www.ki.si/en/life-sciences/l01-laboratory-for-biocomputing-and-bioinformatics/Empirical_Valence_Bond/