

THE LOCAL VIBRATIONAL MODE THEORY: AN EFFICIENT ANALYSIS TOOL FOR THE VIBRATIONAL SPECTROSCOPY COMMUNITY

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The local vibrational mode theory originally introduced by Konkoli and Cremer has become over the past years a versatile tool for extracting important chemical information, hidden in vibrational spectroscopy data caused by the delocalized nature of normal vibrational modes in polyatomic molecules.[1,2]

After a short introduction of the theoretical background and description how local vibrational modes are derived from fundamental vibrational normal modes, we will present three recent examples, elucidating how our tool can help finding answers to open vibrational spectroscopy questions: (i) metal-ligand bonding in heme proteins, such as myoglobin and neuroglobin; (ii) disentanglement of DNA normal modes; and (iii) hydrogen bonding in water clusters and ice.

Finally, we will present the open-source local mode program LModeA which can easily be applied after a routine quantum chemical calculation of vibrational frequencies but also to measured vibrational frequencies, with moderate computational costs.

References:

1. Feature Article: The Local Vibrational Mode Theory and Its Place in the Vibrational Spectroscopy Arena, E. Kraka, M. Quintano, H. W. La Force, J. J. Antonio and M. Freindorf, *J. Phys. Chem. A*, 126, 8781 (2022)
2. Decoding chemical information from vibrational spectroscopy data: Local vibrational mode theory. E. Kraka, W. Zou, and Y. Tao, *WIREs: Comput. Mol. Sci.*, e1480 (2020)