InFemto Research Group

HEAD:

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GROUP MEMBERS:

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BSc student: Jakub Pawlak

RESEARCH PROFILE:

Ultrafast dynamics and local structure in molecular systems by femtosecond pump-probe spectroscopy, molecular dynamics simulations, spontaneous Raman scattering, photoactive materials.

CURRENT RESEARCH ACTIVITIES:

Investigation of coherent response of the medium in femtosecond time resolved spectroscopy. Three time resolved techniques are applied: transient transmission spectroscopy, optical Kerr effect spectroscopy and transient absorption spectroscopy. The first two techniques provide the information on the vibrational dynamics of molecules composing the medium. Applying femtosecond pump pulses we can detect vibrations of frequencies up to 1000 cm^{-1}, which means also low frequency intermolecular vibrations. The third technique detects the dynamics of electronic transitions in molecules.

Our research has recently concentrated on the study of liquid tetrachlorides and trichlorides, their local structures and dynamics. We also build theoretical models describing our experimental results, which allow us to find important molecular parameters responsible for the dynamics of local order in liquids. Below there are some examples of our recent results.

We are developing scientific software for investigation of the local structure and ultrafast dynamics in liquids, based on molecular dynamics simulations. Our software involves calculation of various correlation functions, statistical analysis of hydrogen bond network and several methods of calculating the femtosecond optical Kerr effect signal. The simulations are made in parallel with experiments. Other investigated systems involve for example the methanol-chloroform mixture, which shows an enhanced

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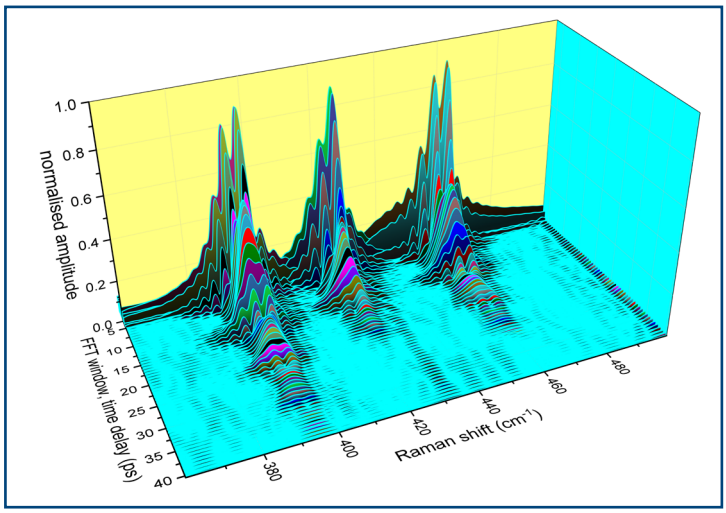
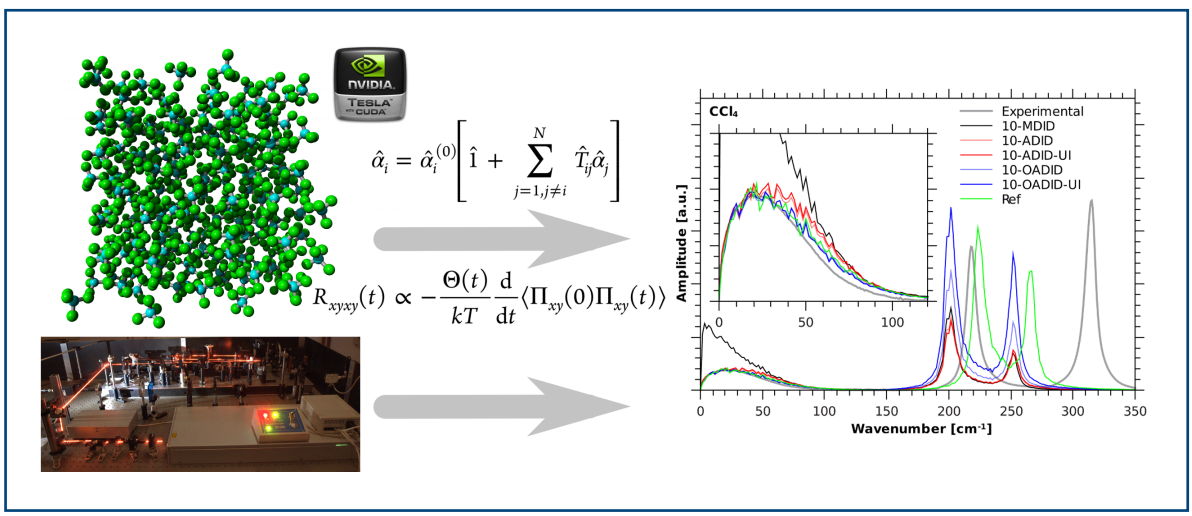


Time evolution of transient transmission spectra of the symmetric stretching vibration in three tetrachlorides. Spectra have been obtained as fast Fourier transforms of time resolved signals. Fine structure of the spectra is connected with the natural abundance of chlorine isotopes ^{35}Cl and ^{37}Cl. It can be well seen due to very high resolution of the spectra.



The femtosecond optical Kerr effect signal is obtained from molecular dynamics simulations and from experiment. Multiple models are validated against the experimental signal to select the best one. The comparison is shown for the Fourier transformed signals. Further analysis of MD trajectoriy allows to distinguish different contributions to the signal.

polarity compared to its components in pure state. This results in a considerably increased solvatochromic effect for some dyes dissolved in this mixture, which is described in terms of synergistic solvation. We are using the same techniques for the mixtures of ionic liquids with simple solvents. These are of great interest due to their potential application as electrolytes in photovoltaic devices. In this study we want to understand the molecular origins of the macroscopic and solvation properties of those mixtures. Recently, the application of organic-inorganic lead trihalide perovskite semiconductors in solar cells gave rise to a new class of solar cells that achieved a power conversion efficiency of over 20%. Many important processes which shape the optical properties of nanostructured semiconductors occur on a femtosecond to nanosecond timescale. To research such fast evolution of photoexcited charge carriers we are using pump-probe transient absorption (TA) and terahertz (THz) spectroscopies with femtosecond resolution. The results of our experiments allow us to decipher the mechanisms behind high overall efficiency of perovskite-based solar cells.

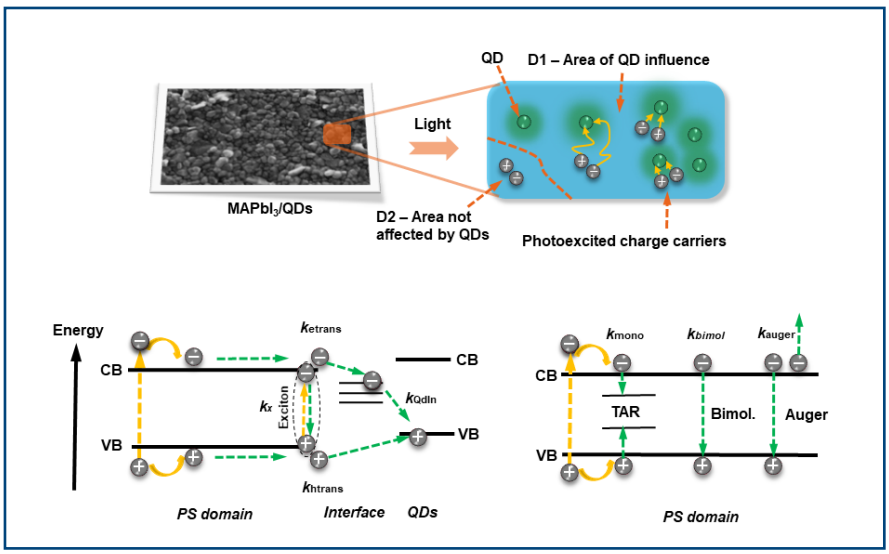


Diagram showing charge carriers migration in MAPbI3/PbS QDs system.

SELECTED PUBLICATIONS:

1. N. Subba, K. Polok, P. Piątkowski, B. Ratajska-Gadomska, R. Biswas, W. Gadomski, P. Sen, Temperature Dependent Ultrafast Solvation Response and Solute Diffusion in Acetamide–Urea Deep Eutectic Solvent, J. Phys. Chem. B. 123(43) (2019) 9212-9221.
2. W. Gadomski, B. Ratajska-Gadomska, K. Polok, Fine structures in Raman spectra of tetrahedral tetrachloride molecules in femtosecond coherent spectroscopy, J. Chem. Phys. 150 (2019) 244505.
3. P. Galar, P. Piątkowski, T.T. Ngo, M. Gutiérrez, I. Mora-Seró, A. Douhal, Perovskite-quantum dots interface: Deciphering its ultrafast charge carrier dynamics, Nano Energy. 49 (2018) 471-480.
4. K. Polok, Simulations of the OKE Response in Simple Liquids Using a Polarizable and a Non-Polarizable Force Field, J. Phys. Chem. B. 122 (2018) 1638.
5. P. Piątkowski, B. Cohen, S. Kazim, S. Ahmad, A. Douhal, How photon pump fluence changes the charge carrier relaxation mechanism in an organic–inorganic hybrid lead triiodide perovskite. Phys. Chem. Chem. Phys. 18 (2016) 27090-27101.
6. P. Piątkowski, B. Cohen, F.J. Ramos, M. di Nunzio, M.K. Nazeeruddin, M. Grätzel, S. Ahmad, A. Douhal, Direct monitoring of ultrafast electron and hole dynamics in perovskite solar cells, Phys. Chem. Chem. Phys. 17 (2015) 14674-14684.
7. K. Polok, W. Gadomski, B. Ratajska-Gadomska, Femtosecond optical Kerr effect setup with signal "live view" for measurements in the solid, liquid and the gas phase, Rev. Sci. Instr. 86 (2015) 103109.
8. P. Piątkowski, C. Martin, M. R. di Nunzio, B. Cohen, S. Pandey, S. Hayse, A. Douhal, Complete Photodynamics of the Efficient YD2-o-C8-Based Solar Cell, J. Phys. Chem. C. 118 (2014) 29674–29687.
9. T. Kardaś, B. Ratajska-Gadomska, A. Lapini, E. Ragnoni, R. Righini, M. Di Donato, P. Foggi, W. Gadomski, Dynamics of the time-resolved stimulated Raman scattering spectrum in presence of transient vibronic inversion of population on the example of optically excited trans-β-apo-8'-carotenal, J. Chem. Phys. 140 (2014) 204312.
10. B. Ratajska-Gadomska, W. Gadomski, Influence of confinement on solvation of ethanol in water studied by Raman spectroscopy, J. Chem. Phys. 133 (2010) 234505.