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RESEARCH ARTICLE

AN APPROACH TO DETERMINING THE PERMITTIVITIES OF ARBITRARY MATERIALS AND THE INTERNAL QUANTUM EFFICIENCY OF EMITTERS

***Guy Francis Mongelli**

Department of Chemical Engineering, Case Western Reserve University, 10900 Euclid Ave., A.W. Smith 116, Cleveland, OH 44120

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ABSTRACT

This manuscript combined several fundamental chemical, physical and mathematical concepts to provide a framework towards molecular simulation of the real and complex refractive index of arbitrary materials may be discerned. Furthermore, it suggests a related method to determine the internal quantum efficiency (IQE) of light emitting diode materials.

Key words:

INTRODUCTION

Recently, several researchers have been focusing on enhancing the internal quantum efficiency and out-coupling efficiency of light emitting diode materials (Patel et al., 2002; Mehta, 2006; Lu, 2002; Nakamura et al., 2006; Peng et al., 2004). Baldo et al. have reported internal quantum efficiencies near 100%. However, the out-coupling efficiency of the best organic light emitting diodes is still at only approximately 80% (Patel et al., 2002; Nakamura et al., 2006). In order to enhance the out-coupling efficiency of OLED technologies studies must seek to modify the angles that makes with respect to surface normal, shifting towards normally emitted light, or otherwise to find high internal quantum efficiency materials which have low refractive indices such as to nullify the critical angle limitation and mitigate Fresnel reflections.

Discussion: An alternative approach

Many scholars have sought to increase the out-coupling efficiency through internal and external device modifications, including scattering particles, micro-lens arrays, the micro-cavity effect, photonic crystals and other methods. Perhaps, however, the method to reach an out-coupling efficiency of near 100% is through the reduction of the refractive index of the organic emitters to 1. Such a proposition requires that the emitting materials have the critical properties that present, common emitters have: they must have a high internal quantum efficiency. Certainly, this stronger requirement will be more difficult to satisfy than has current research. It took over 25 years of global research to obtain high internal quantum efficiency emitting molecules. It could take just as long or longer to solve the suggested problem. The key to the achieving this approach is molecular simulation.

Corresponding author: Guy Francis Mongelli
Department of Chemical Engineering, Case Western Reserve University, 10900 Euclid Ave., A.W. Smith 116, Cleveland, OH 44120

Inter-relating Schrodinger's and Maxwell's Equations

This manuscript suggests that it is possible to simulate the real and complex refractive index of arbitrary materials through inter-relating two sets of fundamental equations in space and time. Those are Maxwell's Equations and Schrodinger's Equations. Consider the orbital structure, number of molecules and their spatial arrangement, and the input EM source as inputs to such a simulation. Perturbations in the E field would be transferred into potential energy as the wave hits the material from an initial vacuum region. Schrodinger's equation re-configures the orbitals to allow light to pass through and the "efficiency" of how the material converts the field to potential energy and back again will dictate k. The speed of the process determines n. That the orbitals reconfigure is an underlying assumption. If they do not reconfigure in a material-specific manner, the author doesnot have a fundamental means by which to explain how different materials have varied n and k, or alternatively first and second dielectric permittivities. There are no good, numerical toolspresently to help determine what the Nature of such optical propagation "transition states" are for arbitrary materials.

The "trick" is to look for which terms in each equation are most readily convertible into energy-like quantities and then finding a way to account for differences in how each equation interacts with energy. This will involve looking at the time-independent Schrodinger equation, and also applying a numerical path integral formulation approach. It is not clear if the macroscopic or microscopic Maxwell's equations are more useful for this computation. Furthermore, whether to use the differential or integral forms (Roundy, 2015). It is possible one set will be required for the time-dependent case and another set for the time-independent case. This approach offers a way to simulate the real and imaginary index of arbitrary

materials to search for high IQE emitters which have a lower index than presently known materials. If we can solve this n-and-k-from-first-principles problem, we should also be able to solve the problem of determining the IQE of an arbitrary material from ab-initio computations. That would involve giving the solid state molecules energy equal to I*V and seeing what their orbital re-configurations are and the states relax. This method might also tell us about the turn-on characteristics from a first principles. Additionally, how the refractive index varies for a given set of lattice parameters for organized materials.

Obstacles

Before such simulations could be achieved, open source Schrodinger's equations solvers must be integrated into open source finite-difference time-domain (FDTD) simulation tools.ORCA[9], GAMESS[10] and MOLCAS[11]are leaders in the former. Meep is the presumptive leader in the latter[12]. Achieving integration and simultaneous solution of these equations will be no small feat.

Conclusion

This manuscript offers new insight on a potential method for the determination of the real and imaginary refractive index from first principles. Furthermore, it suggests that the internal quantum efficiency and turn-on characteristics for OLED devices will also be readily derived once a software package is written to handle the heavy lifting of the numerical computations. Approaching this problem will require contributions from scholars across fields, in electrodynamics – such as the Kurt Busch group[13] and David Roundy group.

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REFERENCES

Aquilante, F. et al. 2016. "Molcas 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table" 37, 5 506-541.

Busch, K. and John, S. 1998. "Photonic band gap formation in certain self-organizing systems" Phys. Rev. E 58, 3896.

Guest, M.F. et al. 2005. "The GAMESS-UK electronic structure package: algorithms, developments and applications" Molecular Physics 103, 6-8 719-747 (2005).

Lu, M.H., Sturn, J.C. 2002. J. Appl. Phys. 91, 595.

Mehta, D.S., Saxena, K. 2006. In: Proceedings of the Ninth Asian Symposium onInformation Display (ASID-06) 198.

Nakamura, T., Fuji, H., Juni, N., Tsutsumi, N. 2006. Opt. Rev. 13, 104.

Nakamura, T., Fuji, H., Juni, N., Tsutsumi, N. 2006. Opt. Rev. 13, 104.

Neese, F. 2012. *"The ORCA program system". Wiley Interdisciplinary Reviews: Computational Molecular Science* ***2****, 1 73–78.*

Oskiooi, A.F. et al. 2010. "MEEP: A flexible free-software package for electromagnetic simulations by the FDTD method" Computer Physics Communications 181, 3 687-702.

Patel, N.K., Cinà, S., Burroughes, J.H. 2002. IEEE J. Select. Top. Quant. Electron. 8,346.

Patel, N.K., Cinà, S., Burroughes, J.H. 2002. IEEE J. Select. Top. Quant. Electron. 8 346.

Peng, H.J., Ho, Y.L., Qiu, C.F., Wong, M., Kwok, H.S. 2004. SID 04 Digest 158.

Pototcshnig, M. et al. 2009. "Time-Domain Simulations of the Nonlinear Maxwell Equations Using Operator-Exponential Methods" IEEE Transactions on Antennas and Propagation 57, 2 475-483.

Roundy, D. et al. 2015. "Experts' understanding of partial derivatives using the partial derivative machine" Phys. Rev. ST Phys. Educ. Res 11, 020126.

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