- *Materials with wide-ranging applications:* The aim is to promote research on the most promising avenues for improving the functionality and performance of existing materials, and the development of new materials with distinctly new or radically improved characteristics.
- *Materials production and transformation processes:* As the production and transformation processes of materials have a major influence on cost and materials properties, research will focus on technologies which can ensure quality, reliability, and cost effectiveness.
- *Sustainable use of materials:* A growing need exists for the development of sustainable technologies. Research will focus on the environmental and safety impact of new materials and on recycling materials.

Conclusion

New and advanced materials are a fundamental and key technology in any advanced society. The development of advanced materials is a horizontal, cross-cutting technology affecting many areas of the economy. The Fifth Framework Programme of the EU recognizes the importance and cross-cutting nature of materials research and will include a specific activity on generic materials research and technological development.

Further information on EU Research Policies can be found on the EU website http://europa.eu.int/pol/rd/en/info.htm and on the CORDIS RTD information service at http://www.cordis.lu/fifth/home.html.

***Edith Cresson**, former prime minister of France (1991–1992), is the Commissioner for Research, Innovation, Education, Training and Youth of the European Commission.*

Letters to the Editor

Effective Mass Approximation Revisited

To the Editor:

In an article in the February 1998 *MRS Bulletin*, p. 35, Alex Zunger gives an overview of the direct diagonalization method (DDM) for calculating the electronic structure of quantum dots, presents some results of that approach, compares them with 6-band effective mass approximation (EMA) calculations and implies the EMA is a general failure. We do not share the author's conclusion. Rather, we remind him that the 6-band EMA has been spectacularly successful in describing absorption,[1] hole burning,[2] and photoluminescence excitation spectra[3,4] in CdSe quantum nanocrystals, has given a quantitative description of the Stokes shift of the resonant photoluminescence and the magnetic field dependence of the fluorescence decay time,[5] and magnetic circular dichroism experiments.[6] The assignment of electronic states based on the EMA provides the foundation for almost every description of electronic structure in quantum dots.[7] The 6-band model, however, is not appropriate for narrow and moderate bandgap semiconductors; rather, one must use its extension to the 8-band EMA[8] which takes the coupling between valence and conduction bands into account. Indeed, we have found that even in narrow gap InAs nanocrystals, this model is very successful in describing transition oscillator strengths and the structure of the absorption spectra.[9] In order to claim accepted standing as a legitimate model for describing the properties of quantum dots, it is encumbent for the DDM to at least show that it produces good physical values for those bulk parameters—including the Kane matrix element—that strongly affect the level structure in these dots.

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Alexander Efros
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Response:

Merv Rosen and Sasha Efros comment that my review article on "Electronic Structure Theory of Semiconductor Quantum Dots"[1] (February special issue) "implies the effective mass approximation (EMA) is a general failure," and that I did not adequately list the successes of the EMA. I regret that within the limited space and scope of a short review paper in the *Bulletin* I could not cite more than four of their articles.

As to the adequacy of the EMA, my research over the past few years had shown me that because the EMA builds into the Hamiltonian the correct physical symmetry of the system at hand, it can achieve good agreement with experiment via judicious selection of its parameters. It thus provides a useful representation and a practical interpolation scheme. However, good agreement with experiment does not always imply good theory. Indeed, some of the (Luttinger-Kane) parameters of the multiband EMA are not physical observables in their own right, but have meaning only in the context of a given, highly simplified model. Thus, these parameters are not "measured." Furthermore, in some cases the EMA parameters are adjusted *de facto* to fit the experiments they claim to explain theoretically. For example, consider $\mathbf{k}\cdot\mathbf{p}$ calculations on CdSe dots: Norris and Bawendi[2] say, "We use standard nonlinear least-squares method to globally fit the experimental data...our fitting routine adjusts three parameters: the Luttinger band parameters γ^1 and γ^2...and the potential barrier for electrons." Efros et al.[3] say, "The position of the quantum size levels are very sensitive to the valence band energy parameter; those used for calculation...give the best description of the CdSe microcrystal absorption spectra." Wind et al.[4] say, "Fig. 1 shows the experimental values...the lines in Fig. 1 have been calculated following a model including the valence mixing....The best correspondence could be obtained [by] choosing a Luttinger parameter $\gamma = 0.38$...." Since the EMA theory is explicitly fit to experiment, it cannot examine the legitimacy of either its successes or its failures.

In fact, by "hard wiring" into the EMA a description of zero-dimensional (0D) quantum dots via very few states drawn from a parametrized three-dimensional (3D) bulk-periodic solid, the model is not systematically extendable to the limit of convergence. It thus cannot be verified or refuted on the basis of its own structure.

It is precisely for these reasons that we developed a systematically extendable and internally verifiable alternative—the direct diagonalization pseudopotential method.[1] By conducting careful, side-by-side comparisons[1, 5, 6] between this converged approach and the equivalent EMA approach, it was possible to examine (and demystify!) the real success of the underlying EMA theory. I find[7] that the EMA is not a general failure. But, when dots that lack periodicity in any of the three dimensions, and exhibit massive band coupling due to low-symmetry, strain, and surface effects, are modeled by using just a handful of fully periodic-like bulk orbitals, something is likely to give.[1, 5, 6] In particular, the EMA fails in describing correctly the order of energy levels in some dot structures, misses many states altogether, overestimates the electron-hole Coulomb energy, misses the long range part of the electron-hole exchange interaction, and fails in describing the important role played by off-Gamma states in the spectroscopy of quantum dots.

Alex Zunger
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Pursuit of Alchemy for What Price?

To the Editor:

Although I have tried hard, I cannot refrain from commenting on the article, "Computational Alchemy: The Search for New Superhard Materials," by David M. Teter that appeared in the January issue of *MRS Bulletin*. The article itself is excellent. It represents a great deal of hard work in forming a database, and it is well written. It raises some very vexatious issues, however. One its own title implies. Is alchemy a suitable scientific pursuit? Another is: Should public taxes support alchemy? A third is: Why don't we have better means for judging the realism of research topics before large amounts of resources are dissipated in their pursuit?

I, for one, have no objection to private funds being spent on alchemy, or almost any other topic. Nor do I object to small amounts of public funds being spent on highly speculative topics. In fact, I think it to be desirable. However, a "companion" study to that of Teter, done by Robert C. DeVries ("Inventory on Innovative Research: The Case of C_3N_4," *Mat. Res. Innovat.* **1** [1997] p. 161) reported that as of about July 1997, the number of papers (starting in about 1984) published regarding "superhard materials" was about 402 with no significant results (consistent with an earlier period of alchemy). This count has probably risen to about 450 by this time. DeVries estimates about three authors per paper. Suppose that, on average, each author spent three months, and that the average cost per month is $10 thousand. Then about $14 million have been spent on this will-o-the-wisp. Not a small amount!

To intensify the pain, the whole pyramid is based on sophistry. The activity started with the notion that the bulk modulus of a solid can be used as an index of its hardness. But it has been known, at least from the time of S.F. Pugh (*Philos. Mag.* **45** [1954] p. 823) that this is not true. Furthermore, the unusual (and probably unique) elastic property of diamond is *not* its bulk modulus, but its shear moduli. And shear moduli are not simply proportional to bulk moduli. This has been well known to researchers in the field and is beautifully confirmed by Teter's data.

In addition, extensive computational work has been done to justify efforts to synthesize a C_3N_4 compound, but a quick perusal of most general chemistry texts indicates that the ground state of the C,N system is cyanogen (C_2N_2), which is a gas at room temperature! This supports the theorem of information theory that computation does *not* produce knowledge; it only processes data. Experiment triumphs!

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