regions of all homologues of M_4-LDH (ref. 8) does not hinder the functional adaptation of each LDH to the temperature conditions it experiences. For the LDHs of low cell temperature species, which must function at low and, in many cases, highly variable temperatures, adaptive reductions in $\Delta G‡$ and $\Delta H‡$ seem to have been achieved by means of increased exergonic exposures of hydrophilic protein groups during the activation step in catalysis. Thus, a higher catalytic efficiency (lower $\Delta G‡$) and a reduced temperature dependency (lower $\Delta H‡$) can both be achieved by evolutionary changes in enzyme structure at regions remote from the active site.

GEORGE N. SOMERO

Scripps Institution of Oceanography, University of California, San Diego, La Jolla, California 92093

PHILIP S. LOW

Department of Chemistry, Purdue University, West Lafayette, Indiana 47907

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Calculated forbidden band gap in periodic protein models indicating them to be insulators

THE idea of electron and hole transport between distant sites in biological macromolecules, especially in fibrous proteins[1] prompted quantum chemists to calculate the forbidden energy band gap in simple periodic protein models[2–7]. Conductivity measurements of several proteins under various conditions indicated a band gap or activation energy (E in the expression for the conductivity $\sigma=\sigma_0 \exp(-E/2kT)$ as function of the temperature T) of the order of 3 eV (refs 8, 9), a value in agreement with the only theoretical energy band gap available at that time (ref. 2). Therefore, the intrinsic mechanism of semiconduction along hydrogen bridges seemed to be well established in 1960. Later, however, both experimentally[10–13] and theoretically the question arose whether the conduction mechanism is really intrinsic. The more refined all-valence-electron quantum chemical calculations[5–7] indicated larger gaps (values in the range 6.1–16.7 eV were reported) than obtained in experiments. Most interestingly the calculation of Morokuma[5] at complete-neglect-of-differential-overlap level showed that in a polyglycine chain the bandgap was not too sensitive to the changes of the chain's conformation: in conformers with appreciable H-bonding the gap found was slightly larger than in the β-sheet conformation. This latter finding pointed out the very small influence of H-bonds on the forbidden gap of periodic protein models. These semi-empirical calculation methods were designed for molecular purposes and there is still little known of their applicability to the calculation of the gap in crystals and polymers[14,19]. Thus we describe here use of the more reliable non-empirical (*'ab initio'*) crystal orbital method[15] to calculate the band gap in a most simple polypeptide model β-polyglycine.

We used an STO-3G atomic orbital basis set[16]. After evaluation of all integrals[17], as usual in molecular *ab initio* calculations, we performed a self-consistent-field calculation using a first neighbour's interaction approximation. This highly sophisticated calculation resulted in a gap of 19.23 eV, the largest value obtained so far. Although larger numbers of included neighbours, basis set enlargement and correlation corrections may reduce this value by several eV, it seems impossible to reduce this value to the vicinity of the experimental gap. We may conclude therefore, that the intrinsic mechanism in a periodic protein model can be ruled out. Absolutely pure periodic proteins are thus good insulators. This conclusion will probably remain valid even in presence of orientational randomness of the constituent units. A set of aperiodic side chains, however, may serve as impurity centres, which support extrinsic type conduction.

The lowest energy optical transition of the electron system corresponds to the formation of excitons within the forbidden gap rather than to free electrons and holes. The order of magnitude of the energy of these excitons is expected to be 6–8 eV on the basis of the first electronic transition energies of small peptides[18]. Although this value is much larger than the experimental E it is necesarily smaller than the theoretical band-to-band gap found in our calculation.

Some technical details, which are of interest to specialists only, will be given elsewhere.

M. KERTESZ

Central Research Institute for Chemistry, 1525 Budapest, Pf. 17, Hungary

J. KOLLER
A. AŻMAN

Chemical Institute B. Kidric, 61001 Ljubljana, Pp. 380, Yugoslavia

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Errata

The caption for the cover picture for *Nature*, vol. **264**, no. 5583 should have read: Microtubules polymerised *in vitro* and stained with the PAP-procedure with omission of the anti-tubulin antibody solution.

In the Statement published in *Nature*, vol. **265**, p. 764, the first line of the last paragraph of the letter from B. Hamprecht should have read 'The data on cyclic GMP were'. . . .

In the article 'Low temperature specific heat of glasses and amorphous solids' by P. R. Couchman, C. L. Reynolds, Jr, & R. M. J. Cotterill, *Nature*, **264**, 534 (1976), the units for G in paragraph three are dyn cm^{-2}, not dyn cm^{-3}.

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