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## A Novel Design of Photonic Band Gap by F.W.C.I.P Method

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**Abstract:** The study of the photonic band structure of periodic structures is an important subject in photonics. In this paper, a novel method is proposed for the calculation of the photonic band structure of periodic structures. The method is based on the finite difference method (FDM) and the plane wave expansion method (PWE). The results show that the proposed method is more accurate and efficient than the other methods. The method is applied to the calculation of the photonic band structure of a one-dimensional photonic crystal. The results show that the proposed method is more accurate and efficient than the other methods.

**1. INTRODUCTION**  
 Photonic crystals (PCs) are periodic structures of dielectric materials. They are used in a wide range of applications, such as waveguides, filters, and lasers. The study of the photonic band structure of PCs is an important subject in photonics. In this paper, a novel method is proposed for the calculation of the photonic band structure of periodic structures. The method is based on the finite difference method (FDM) and the plane wave expansion method (PWE). The results show that the proposed method is more accurate and efficient than the other methods.

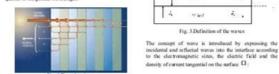


Fig. 1. FDM grid

The wave number is given by  $k = \frac{2\pi}{\lambda}$ , where  $\lambda$  is the wavelength of the light. The wave number is given by  $k = \frac{2\pi}{\lambda}$ , where  $\lambda$  is the wavelength of the light. The wave number is given by  $k = \frac{2\pi}{\lambda}$ , where  $\lambda$  is the wavelength of the light.



Fig. 2. Definition of the wave

The number of waves is calculated by  $N = \frac{L}{\lambda}$ , where  $L$  is the length of the structure. The number of waves is calculated by  $N = \frac{L}{\lambda}$ , where  $L$  is the length of the structure. The number of waves is calculated by  $N = \frac{L}{\lambda}$ , where  $L$  is the length of the structure.

## A climbing image nudged elastic band method for finding saddle points and minimum energy paths

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A modification of the nudged elastic band method for finding minimum energy paths is presented. One of the images is made to climb up along the elastic band to converge rigorously on the highest saddle point. Also, variable spring constants are used to increase the density of images near the top of the energy barrier to get an improved estimate of the reaction coordinate near the saddle point. Applications to CH<sub>4</sub> dissociative adsorption on Ir(111) and H<sub>2</sub> on Si(100) using plane wave based density functional theory are presented. © 2000 American Institute of Physics.

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### 1. INTRODUCTION

An important problem in theoretical chemistry and condensed matter physics is the calculation of transition rates, for example rates of chemical reactions or diffusion events. Most often, it is sufficient to treat the motion of the atoms using classical mechanics, but the transitions of interest are typically many orders of magnitude slower than vibrations of the atoms, so a direct simulation of the classical dynamics is not feasible. For a process with typical, low activation energy of 0.5 eV, the computer time required to simulate a classical trajectory long enough that a single transition event can be expected to occur is on the order of 10<sup>10</sup> years on present day computers. This "rare event" problem is devastating for direct dynamical simulations, but makes it possible to obtain accurate estimates of transition rates using a purely statistical approach, namely, transition state theory (TST).<sup>1-3</sup> Apart from the Born-Oppenheimer approximation, TST relies on two basic assumptions: (a) the rate is slow enough that a Boltzmann distribution is established and maintained in the reactant state and (b) a dividing surface of dimensionality D-1, where D is the number degrees of freedom in the system, can be identified such that a reacting trajectory going from the initial state to the final state only crosses the dividing surface once. The dividing surface must, therefore, represent a bottleneck for the transition.

Since atoms in crystals are usually tightly packed and the typical temperature of interest is low compared with the melting temperature, the harmonic approximation to TST (HTST) can typically be used in studies of diffusion and reactions in crystals or at crystal surfaces.<sup>4</sup> This greatly simplifies the problem of estimating the rates. The search for the optimal transition state then becomes a search for the lowest few saddle points at the edge of the potential energy basin corresponding to the initial state. The rate constant for transition through the region around each one of the saddle

$$k_{TST} = \frac{\int_{\Omega} \prod_{i=1}^D \nu_i e^{-E^{\ddagger}/k_B T} e^{-E^{\ddagger}/k_B T} d\Omega}{\int_{\Omega} e^{-E^{\ddagger}/k_B T} d\Omega} \quad (1)$$

Here,  $E^{\ddagger}$  is the energy of the saddle point,  $E^{\ddagger}$  is the local potential energy minimum corresponding to the initial state, and the  $\nu_i$  are the corresponding normal mode frequencies. The symbol  $\Omega$  refers to the saddle point. All the quantities can be evaluated from the potential energy surface, at zero temperature, but entropic effects are included through the harmonic approximation. The most challenging part in this calculation is the search for the relevant saddle point.

A path connecting the initial and final states that typically has the greatest statistical weight is the minimum energy path (MEP). At any point along the path, the force acting on the atoms is only pointing along the path. The energy is stationary for any perpendicular degree of freedom. The maxima on the MEP are saddle points on the potential energy surface. The relative distance along the MEP is a natural choice for a reaction coordinate, and at the saddle point the direction of the reaction coordinate is given by the normal mode eigenvector corresponding to negative curvature.

The MEP often has one or more minima in addition to the maxima at the initial and final states. These correspond to stable intermediate configurations. The MEP will then have two or more maxima, each one corresponding to a saddle point. Assuming a Boltzmann population is reached for the intermediate (metastable) configurations, the overall rate is determined by the highest saddle point. It is, therefore, not sufficient to find a saddle point. One needs to have a good enough estimate of the shape of the MEP to be able to assign the highest saddle point as  $\ddagger$  in Eq. (1) in order to get an accurate estimate of the rate.

## Trumpet Major Scales and Arpeggios In Range Order

(E) F# Major

(F) G Major

(Gb) Ab Major

(G) A Major





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