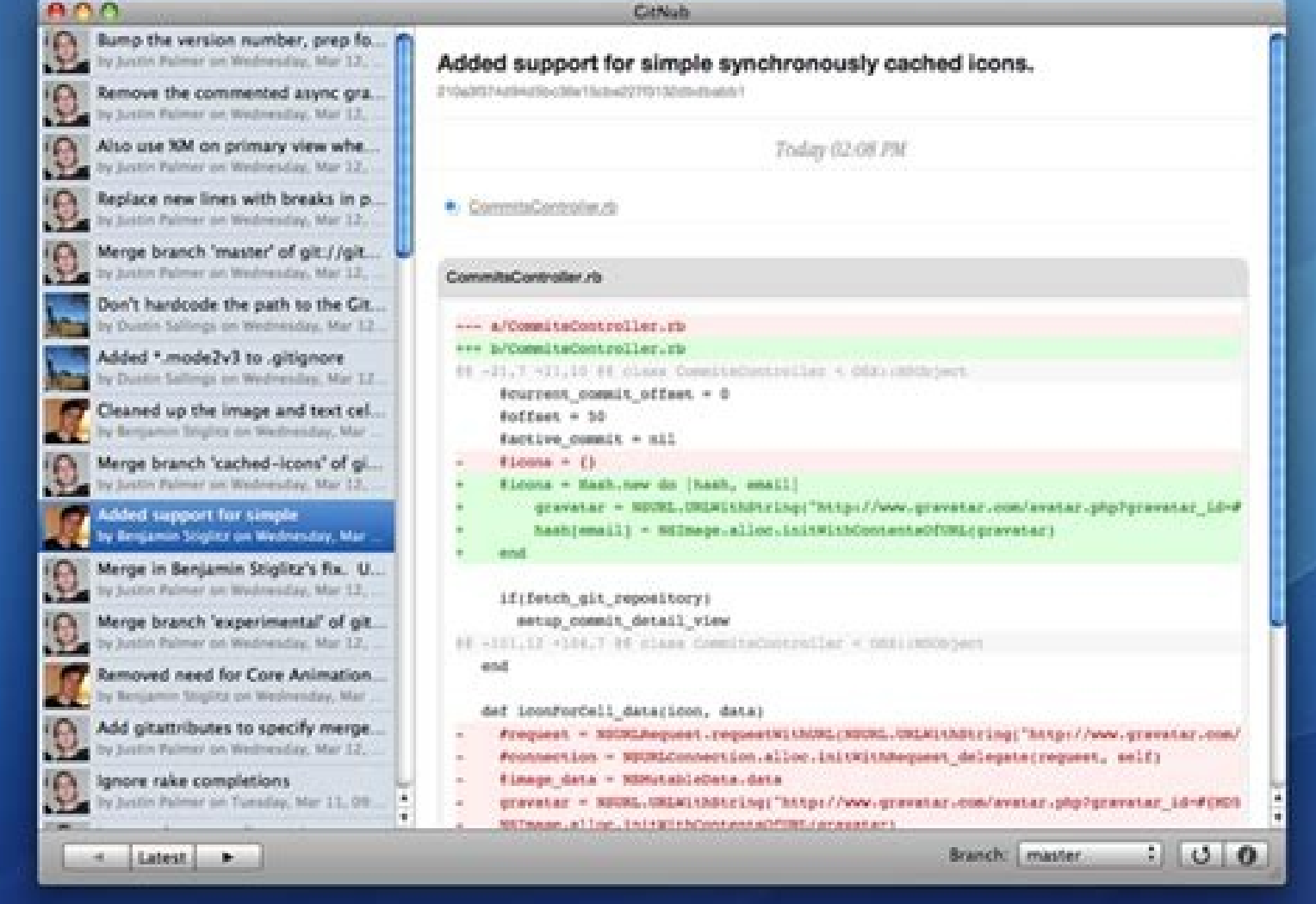


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## Computer modelling of point defects in $ABO_3$ perovskites and MgO

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### Abstract

We present results for basic intrinsic defects: F-type electron centers (O vacancy which trapped one or two electrons) and hole polarons bound to Mg or K vacancy in ionic MgO and partly covalent  $KNbO_3$  perovskite, respectively. We demonstrate that a considerable covalency of the perovskite chemical bonding makes the F-type centers therein much more similar to defects in partly-covalent quartz-type oxides rather than the conventional F centers in alkali halides and ionic MgO. Both one-site (atomic) and two-site (molecular) polarons are expected to coexist in  $KNbO_3$ , characterized by close absorption energies. Our calculations confirm existence of the self-trapped electron polarons in  $KNbO_3$ ,  $KTaO_3$ ,  $BaTiO_3$  and  $PbTiO_3$  crystals. The self-trapped electron is mostly localized on B-type ion due to a combination of breathing and Jahn–Teller modes of nearest six oxygen ion displacements. The relevant lattice relaxation energies are typically 0.2–0.3 eV, whereas the optical absorption energies 0.7–0.8 eV, respectively. According to our calculations, the absorption energy of a bound electron polaron in  $KNbO_3$ , by 0.1 eV exceeds that for the self-trapped electron polaron and equals 0.88 eV.  
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PAICS: 71.15.Ag; 71.35.Cc; 71.38.Hi  
Keywords:  $ABO_3$  perovskites; F centers; Electron polarons; Hole polarons; Quantum chemical calculations

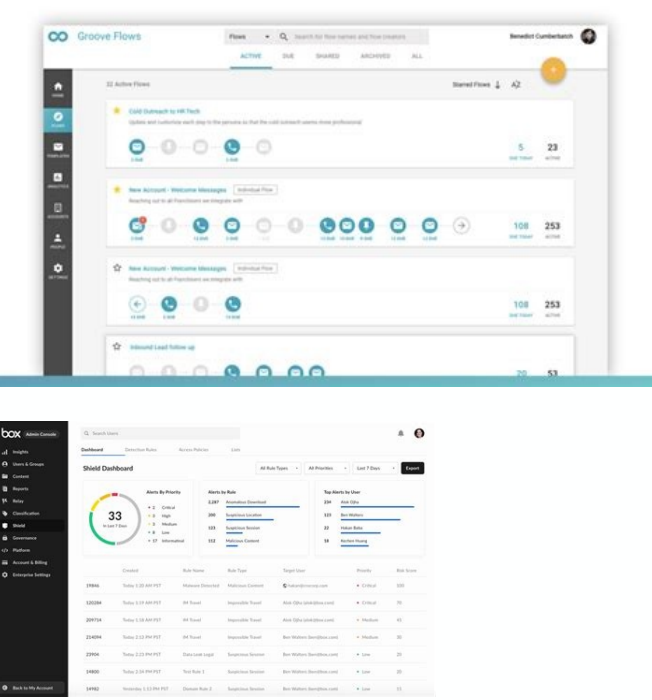
### 1. Introduction

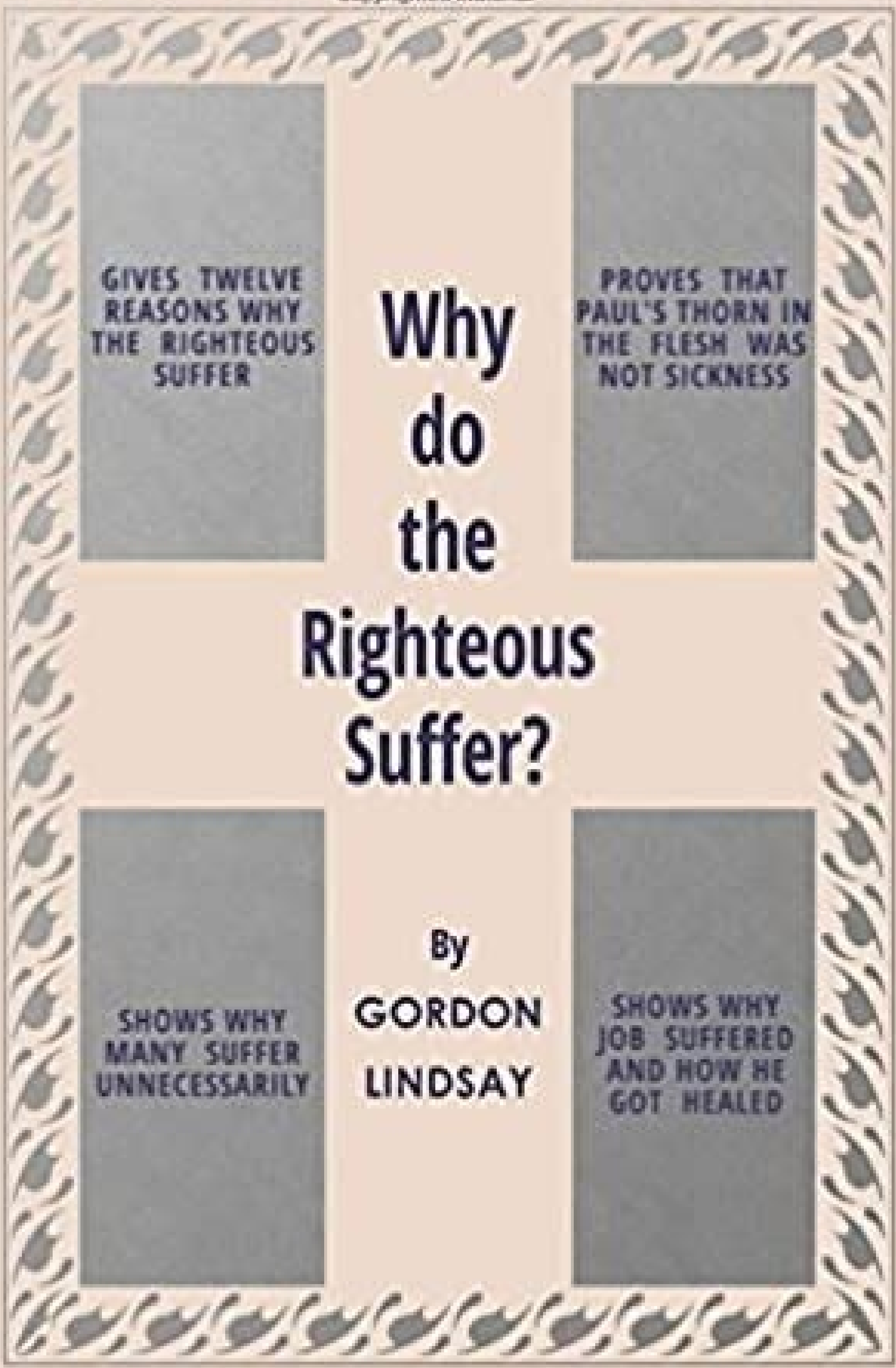
Most of real crystals are non-stoichiometric and thus contain along with impurities large concentrations of intrinsic defects—vacancies. Oxygen vacancies are known to give rise to  $F^+$  and  $F^0$  centers (vacancy which trapped one or two electrons, respectively) [1]. The properties of F-type centers in ionic oxides like MgO and  $\alpha-Al_2O_3$  are well studied, unlike  $KNbO_3$  perovskite where up to now there exists only a tentative assignment of the electron-induced absorption band at 2.7 eV to the F-type centers [2]. In its turn, cation vacancies are able to trap radiation-induced holes. Thus, in irradiated MgO a cation vacancy is known to trap one or two holes giving rise to the  $V^+$  and  $V^{2+}$  centers [1,3] called bound hole polaron and

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chips,[d] was thereby described as an iAPX 86 system.[6][e] There were also terms iRMX (for operating systems), iSBC (for single-board computers), and iSBX (for multimodule boards based on the 8086-architecture), all together under the heading Microsystem 80.[7][8] However, this naming scheme was quite temporary, lasting for a few years  
during the early 1980s.[f] Although the 8086 was primarily developed for embedded systems and small multi-user or single-user computers, largely as a response to the successful 8080-compatible Zilog Z80,[9] the x86 line soon grew in features and processing power. Today, x86 is ubiquitous in both stationary and portable personal computers, and is  
also used in midrange computers, workstations, servers, and most new supercomputer clusters of the TOP500 list. A large amount of software, including a large list of x86 operating systems are using x86-based hardware. Modern x86 is relatively uncommon in embedded systems, however, and small low power applications (using tiny batteries), and  
low-cost microprocessor markets, such as home appliances and toys, lack significant x86 presence.[g] Simple 8- and 16-bit based architectures are common here, although the x86-compatible VIA C7, VIA Nano, AMD's Geode, Athlon Neo and Intel Atom are examples of 32- and 64-bit designs used in some relatively low-power and low-cost segments.  
There have been several attempts, including by Intel, to end the market dominance of the "inelegant" x86 architecture designed directly from the first simple 8-bit microprocessors. Examples of this are the iAPX 432 (a project originally named the Intel 8800[10]), the Intel 960, Intel 860 and the Intel/Hewlett-Packard Itanium architecture. However,  
the continuous refinement of x86 microarchitectures, circuitry and The manufacture would make it difficult to replace X86 in many segments. The X86 Extension of 64 Bits of AMD (which Intel finally responded with a compatible design) [11] and the scalability of the X86 chips in the form of modern multinoã cpu, is underlining x86 as an example of  
how refinement the refinement Continuous of the established industry Standards can resist the competition of completely new architectures. [12] Chronology This article needs additional quotes for verification. Help improve this article by adding appointments to reliable sources. The not warned material can be challenged and eliminated. Sources.  
The processors models and the series of models that implement various architectures in the X86 family are listed below. Each linen line is characterized by processing micro -architectures significantly improved or commercially successful. Chronology of the X86 processors was Introduction , IBM PC/ IBM/ IBM PC/ XT (8088) 1982 Intel 80186, Intel  
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CX5X86CYRIX 6x86/MX (1997)/MII (1998) Examinity Dynamics 6 (PAE, A e aju-op translation) 1995 ## ##### The native architecture of the X86-64 processors: which resides in the 64-bit mode, lacks access mode in segmentation, presenting space of 64-bit architectural  
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