

Stefan K. Estreicher

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May 6, 1952 Unremarkable birth in Neuchâtel (Switzerland) punctuated by crying (me) and relief (mom).
1982 PhD in theoretical physics, University of Zürich, under Peter F. Meier and Armin Thellung.
1983-1986 Postdoc at Rice University, for Tom L. Estle.
fall 1986 Texas Tech University (Physics): assistant Professor.
 1991: associate Professor; 1996: Professor; 2000 P.W. Horn Distinguished Professor.
1997 Fellow, American Physical Society
2001 Alexander von Humboldt's Friedrich Wilhelm Bessel research prize (Germany)
2006 Fellow, Institute of Physics (UK)
2012 Scientist of the Year, ARCS (Lubbock chapter)
2018-2024 Spokesperson (elected) of the Horn Distinguished Professors at Texas Tech University.

Numbers

Plenary and invited conference talks	57 (physics), 10 (history of wine)
Invited seminars and colloquia	106
Publications	221
Citations / h-index / i10-index	7,580 / 50 / 131 as of July, 2026

Service

Chair, 2002 Gordon Research Conference on *Point and Line Defects in Semiconductors*
Co-chair, 2007 *International Conference on Defects in Semiconductors* (ICDS-24)
Co-organizer of multiple symposia at APS, MRS, and E-MRS meetings
Elected to the international advisory committee of the ICDS (2005-2015)
Acting chair, chair, then chair-elect of the steering committee of the ICDS (2009-2015)
Proceedings editor and guest editor (Journal of Applied Physics): ICDS-24, ICDS-25, ICDS-26, and ICPS-32

Claims to fame

At the Max-Planck Institute in Stuttgart, Joerg Weber and I were looking for something edible at the dreaded 'Mensa' (cafeteria). We found a yogurt-like substance called 'quark' and published that discovery:
S.K. Estreicher, J. Weber, **Ann. Improb. Res.** **II/1**, 20 (1996): *The 7th quark: A challenge to the standard model?*

I am co-author on a paper with Steven Chu, Stephen W. Hawking, Steven Weinberg (+ 439 others): **Ann. Improb. Res.** **10**, 24 (2004): *The Morphology of Steve*. This is about scientists named Steve, Stephen, Stefan, etc. The 443 co-authors found out about it after publication.

I slept in the same bed as Her Royal Highness Elizabeth II, Queen of England: my host at Trinity College (Cambridge) set me up in the 'ultimate guestroom' – the suite where the Queen stayed when visiting. The bed looks (and feels) like it dates back to William The Conqueror. Thus, the Queen and I coincided in space but not in time - which, all agree, is best.

History of wine

This hobby dates back to the mid 70's with a 1949 Richebourg, a wine that grabs your attention: I started to read... I gave talks on the history of wine in California, Texas, South Africa, Sicily, England, China, the Republic of Georgia, Spain, and the Global Physics Summit in March, 2024. I wrote a forgettable book (*Wine: from Neolithic times to the 21st century*, Algora NY 2006). It involved considerable and unwanted interference by editors who re-wrote parts of my text, ignored corrections, and rushed to print. More importantly:

A brief history of wine in Spain, **European Review** **21**, 209-239 (2013)

A brief history of wine in South Africa, **European Review** **22**, 504-537 (2014)

The beginning of wine and viticulture, **Physica Status Solidi c** **14**, 1700008/1-5 (2017)*

this may well be the only history of wine paper published in a physics journal

Wine, The Encyclopedia of Ancient History (Wiley Blackwell 2015, updated 2018, 6 pages)

Wine and France, a brief history, **European Review** **31**, 91-179 (2023) - open access

Wine and Portugal, a brief history, **European Review** **33**, 38-129 (2025) - open access

My next book, *Milestones in the History of Wine*, is in preparation.

Research

1. Heat flow and defects

Energy propagates in materials via electrons, phonons, and other carriers such as magnons. The focus here is on phonons which dominate in dielectrics and low-doped semiconductors. In 1929, Rudolf Peierls described the interactions between phonons and defects in terms of 'lattice waves' scattering off 'lattice imperfections'. After WWII, this became phonon scattering. Today, textbooks and research papers talk about phonon scattering by impurities, surfaces, interfaces, etc. Phonons have become quasi-particles which propagate, carrying quanta of vibrational energy. Some even claim that phonons are bosons, hence fundamental particles.

The results of our first-principles calculations are at odds with the (empirical) phonon-scattering picture. Further, phonons cannot be bosons (see 1f below). Our ideas received considerable pushback, sometimes bordering on hostility. Galileo Galilei was the first to realize the concept of inertia. In the present case, people refuse to change the way they have been thinking for decades. Yet, I suspect that (some of) our views are correct.

a) Supercell preparation: Conventional molecular-dynamics (MD) simulations at a temperature T_0 begin with a Maxwell-Boltzmann distribution of nuclear velocities corresponding to T_0 with all the nuclei at their equilibrium site at the time $t=0$. This is simple, but the MD run begins with zero potential energy: all the vibrational modes are exactly in phase, an unphysical situation. As the MD run begins, all the nuclei lose then gain kinetic energy together and the temperature fluctuations ΔT are comparable to T_0 . Their amplitude must be reduced with a thermostat and extensive 'thermalization' runs are required for the system to reach a reasonable steady-state. Phonon coupling cannot be studied far from the steady state because (i) the fluctuations are larger than many phonon energies and (ii) the oscillators couple to the thermostat much faster than to each other. The need for thermostats and long thermalization runs *entirely* results from the modes being in phase at $t=0$.

My group (especially D. West) developed a new way to prepare the supercell at $t=0$. No thermostat is used. ΔT is constant with time starting with MD step 1 and can be made as small as desired. This was used to calculate the *vibrational lifetimes* of defect-related modes; *thermal conductivities* of systems containing defects; *heat-flow interactions* with surfaces and interfaces; and the temperature dependence of the *Kapitza resistance*. We predict how interfaces can be used to control the flow of heat in various temperature windows.

Supercell preparation: we use the eigenvectors of the dynamical matrix to initiate the system in a combination of normal modes with random distributions of mode phases and energies. No thermostat is used. The magnitude of ΔT is very small starting with MD step 1. For a supercell containing ~ 200 atoms, averaging the MD runs over ~ 30 initial random distributions of mode phases and energies (all corresponding to the same macrostate) produces ΔT of the order of 1% of the background temperature (our record is $\Delta T=0.15\text{K}$ at 125K). T.M. Gibbons, M.B. Bebek, By. Kang, C.M. Stanley, S.K. Estreicher, **J. Appl. Phys.** **118**, 085103 (2015)

b) Vibrational lifetimes: When a normal vibrational mode is excited above the background temperature, it decays as $\exp(-t/\tau)$ by coupling to lower-frequency modes. Many impurity-related lifetimes have been measured by transient-bleaching spectroscopy: the lifetimes of similar Si-H stretch modes sometimes differed by two orders of magnitude or exhibited huge isotope effects. Supercell preparation allowed us to excite the specific mode of interest and then watch it decay while monitoring the energy and amplitude of all the other normal modes in the system. We explained over two dozen experimental results (sometimes with their temperature dependence), including the weird isotope effects. Supercell preparation works quantitatively.

K.K. Kohli, G. Davies, N.Q. Vinh, D. West, S.K. Estreicher, T. Gregorkiewicz, **Phys. Rev. Lett.** **96**, 225503 (2006)
D. West and S.K. Estreicher, **Phys. Rev. Lett.** **96**, 115504 (2006) and **Phys. Rev. B** **75**, 075206 (2007)
D. West, S.K. Estreicher, T.M. Gibbons, S.K. Estreicher, K. Potter, F. Bekisli, M. Stavola, **Phys. Rev. B** **87**, 115207 (2013)

c) Phonon-defect interactions: Gordon Davies (King's College London) referred to the long vibrational lifetimes of impurity-related modes as 'phonon trapping'. But we soon realized that this phenomenon was not restricted to high-frequency impurity-related modes. The normal modes of materials include bulk-related modes (host crystal) which are delocalized in space and have short lifetimes (~one period of oscillation) and defect-related modes which are localized in space and have long lifetimes (dozens or hundreds of periods of oscillation). We named the latter 'Spatially-Localized Modes' (SLMs). Experimentally, some of them are seen by FTIR or Raman spectroscopy, while others show up as low-frequency phonon sidebands in PL spectra.

Whenever heat flows through a material and encounters a defect, some energy traps in SLMs and remains there for a relatively long time. These excited SLMs finally decays into bulk modes but that decay does not correlate with the origin of the excitation but with the availability of receiving modes. Thus, impurities (even isotopes) reduce heat flow because some energy remains trapped at the impurity for a meaningful length of time. Defects act like tiny 'sponges' of energy, not like scattering centers.

S.K. Estreicher, T.M. Gibbons, By. Kang, M.B. Bebek, **J. Appl. Phys.** **115**, 012012 (2014)
S.K. Estreicher, T.M. Gibbons, M.B. Bebek, **J. Appl. Phys.** **117**, 112801 (2015)

d) Surfaces: Surface-related vibrational modes are SLMs. Their frequencies are different from those of bulk modes. For a H-saturated Si nanowire, the Si-H stretch modes ($\sim 2,000\text{cm}^{-1}$) are much too high to be thermally excited but the wag modes ($\sim 900\text{cm}^{-1}$) can be. When a temperature gradient is set up, bulk modes and some surface wag modes are excited. The heat propagates quickly in the bulk while the fraction of the heat trapped on the surface propagates much slower, as resonant coupling between neighboring Si-H wag modes goes back and forth, just like coupled pendulums exchanging energy. The key point here is that there is simply no interaction between surface SLMs and bulk modes: their frequencies are too far apart. The decay of a surface mode into bulk modes involves slow two-phonon processes, as does the excitation of one surface mode starting with two bulk modes. Bulk and surface oscillators do not couple, much less scatter off each other. Surfaces reduce heat flow because one has to wait for the slower surface contribution to arrive before thermal equilibrium is achieved. By. Kang, S.K. Estreicher, **Phys. Rev. B** **89**, 155409 (2014)

e) Interfaces: Consider the interface between materials A and B. On one side, there are A-A vibrational modes, on the other side there are B-B modes. But at the interface there are A-B modes: the SLMs. The system starts at some temperature T_0 and you set up a T gradient in the A region. Heat propagates in material A, hits the interface, and some SLMs trap phonons. The outcome depends on how these SLMs decay. If the A atoms are lighter than the B atoms, then the modes on the A side have higher frequencies than those on the B side. The excited interface SLMs will decay mostly into B-B modes because there are many more low-frequency modes on the B side than on the A side. Then, heat easily flows across the interface. On the other hand, if the A atoms are heavier than the B atoms, then the heat trapped in SLMs will decay back toward the A side because most of the receiving modes are there. As a result, heat accumulates on the A side near the interface, creating the large T discontinuity at the surface associated with the *Kapitza resistance* R_K . Slow two-phonon interactions are required for heat to move across the interface to the B side.

The R_K of the A|B interface depends on the temperature window and on which way heat propagates. When going from a lighter material toward a heavier one, the resistance should be very small. When going from a heavier toward a lighter material, this resistance is large and a step-like T dependence appears. At low T , the SLMs are too high in frequency to be resonantly excited and heat bounces back; at higher T , more heat traps at the interface and starts moving across the interface; at higher T still, more of the higher-frequency modes on the lighter side become excited, heat flows easier, and R_K drops.

M.B. Bebek, C.M. Stanley, T.M. Gibbons, S.K. Estreicher, **Sci. Rep.** **6**, 32150 (2016)
C.M. Stanley and S.K. Estreicher, *Phys. Stat. Sol. A* **2018**, 1800428/1-9 (DOI: 10.1002/pssa.201800428)

f) Phonons as quasi particles: Photons are quanta of electromagnetic energy $\hbar\omega$. Since the electromagnetic field has a Poynting vector, photons have real-space momentum and angular momentum. On the other hand,

phonons are quanta of vibrational energy $\hbar\omega$ associated with specific normal vibrational modes (VMs). There is no Poynting vector. As quantum oscillators couple to each other, phonons disappear in some VMs and new phonons appear in different VMs: there is no such thing as one phonon ‘moving’ through the material or hopping from one oscillator to another: the transfer of energy between VMs involves different phonons. In this process, the center of mass of the oscillation moves because different oscillators are excited. But *in real space*, phonons are not propagating particles.

Phonons have no spin but this does not imply that they are bosons with spin zero. Indeed, one fundamental property of bosons is that you can put as many of them as you wish in the same energy state. Place three bosons in the ground state of a harmonic potential and the total energy is $3\hbar\omega/2$. But if you add three phonons to the same potential, you get $7\hbar\omega/2$. You cannot put even a single phonon in the ground state! What type of boson does that? Note that expanding the denominator of the Bose-Einstein distribution function gives the same population number n as the harmonic oscillator $E = k_B T = (n+1/2)\hbar\omega$, but for the factor $1/2$ which is irrelevant when n is large.

2. Hydrogen in semiconductors

I performed the first ab-initio calculations that included geometry optimizations for defects in semiconductors: neutral H in c-C and Si. They revealed that the fully relaxed Si-Si bond-centered (bc) site is the minimum of the total energy. A few years later, Van de Walle *et al.* showed that the stable charge states are H_{bc}^+ and H_T^- .

T.L. Estle, S.K. Estreicher, D.S. Marynick, **Hyp. Inter.** **32**, 637 (1986) and **Phys. Rev. Lett.** **58**, 1547 (1987)

S.K. Estreicher, **Phys. Rev. B** **36**, 9122 (1987). For a review, see S.K. Estreicher, **Mat. Sci. Engr. Rep.** **14**, 319-412 (1995)

This work was followed by many studies related to H interactions with a wide range of impurities and defects in Si and other materials, including the curious reorientation of the H-P pair in Si:

S.K. Estreicher, C.H. Seager, R.A. Anderson, **Appl. Phys. Lett.** **59**, 1773 (1991)

S.K. Estreicher, R. Jones, **Appl. Phys. Lett.** **64**, 1670 (1994)

C.H. Seager, R.A. Anderson, S.K. Estreicher, **Phys. Rev. Lett.** **74**, 4565 (1995)

My group also did a lot of work on the H_2 molecule in Si and its interactions with radiation damage:

S.K. Estreicher, J.L. Hastings, P.A. Fedders, **Phys. Rev. B** **57**, R12663 (1998) and **Phys. Rev. Lett.** **82**, 815 (1999)

S.K. Estreicher, K. Wells, P.A. Fedders, P. Ordejón, **J. Phys: Cond. Matter** **13**, 62 (2001)

S.K. Estreicher, **Acta Phys. Polon. A** **102**, 403 (2002): *The H_2 molecule in semiconductors: an angel in GaAs, a devil in Si*

3. Transition-metal impurities, migration paths and activation energies

Transition metals are ubiquitous and unwanted impurities. We studied Ti, V, Fe, Co, Ni, Cu, and Ag: migration barriers, electrical and optical activity, interactions with impurities, etc.

D.E. Woon, D.S. Marynick, S.K. Estreicher, **Phys. Rev. B** **45**, 13383 (1992) and J. Lindroos, D.P. Fenning, D. Backlund, E. Verlage, A. Gorgulla, S.K. Estreicher, H. Savin, T. Buonassisi, **J. Appl. Phys.** **113**, 204906 (2013)

D. West, S.K. Estreicher, S. Knack, J. Weber, **Phys. Rev. B** **68**, 035210 (2003)

S.K. Estreicher, M. Sanati, N. Gonzalez Szwacki, **Phys. Rev. B** **77**, 125214 (2008)

D.J. Backlund and S.K. Estreicher, **Phys. Rev. B** **82**, 1155208 (2010) and **Phys. Rev. B** **81**, 235213 (2010)

A. Carvalho, D.J. Backlund, S.K. Estreicher, **Phys. Rev. B** **84**, 155322 (2011)

S.K. Estreicher, D.J. Backlund, C. Carbogno, M. Scheffler, **Angew. Chemie** **50**, 10221 (2011)

D.J. Backlund, T.M. Gibbons, S.K. Estreicher, **Phys. Rev. B** **94**, 195210 (2016)

T.M. Gibbons, D.J. Backlund, S.K. Estreicher, **J. Appl. Phys.** **121**, 045704 (2017)

T.M. Vincent, S.K. Estreicher, J. Weber, W. Kolkovsky, N. Yarykin, **J. Appl. Phys.** **127**, 085704 (2020)

T.M. Vincent and S.K. Estreicher, **J. Appl. Phys.** **128**, 155703 (2020)

4. Other contributions

a) Thermal properties: entropy contributions, specific heats, Debye temperature in c-C, Si, Ge, and GaN:

S.K. Estreicher, M. Sanati, D. West, F. Ruymgaart, **Phys. Rev. B** **70**, 125209 (2004)

M. Sanati, S.K. Estreicher, M. Cardona, **Sol. St. Commun.** **131**, 229 (2004)

M. Sanati, S.K. Estreicher, **J. Phys: Cond. Matter** **16**, L327 (2004) and **Phys. Rev. B** **72**, 165206 (2005)

R.K. Kremer, M. Cardona, E. Schmitt, J. Blumm, S.K. Estreicher, M. Sanati, M. Bockowski, I. Grzegory, T. Suski, A. Jezowski, **Phys. Rev. B** **72**, 075209 (2005)

M. Cardona, R.K. Kremer, M. Sanati, S.K. Estreicher, T.R. Anthony, **Sol. St. Commun.** **133**, 465 (2005)

b) The hexavacancy in Si: The most stable of the small vacancy clusters in Si is the hexavacancy, V_6 , a missing hexagonal ring of Si atoms. It reconstructs so well that it is electrically inactive, but is a strong gettering center: S.K. Estreicher, J.L. Hastings, P.A. Fedders, **Appl. Phys. Lett.** **70**, 432 (1997) and **Phys. Rev. B** **56**, 10215 (1997)
B. Hourahine, R. Jones, A.N. Safonov, S. Öberg, P.R. Briddon, S.K. Estreicher, **Phys. Rev. B** **61**, 12594 (2000)

c) Early work on C_{60} : Buckyballs (C_{60}) are molecules where the C atoms are arranged at the nodes of a soccer-ball-like sphere. Rick Smalley discovered it by mass spectrometry while I was at Rice University. I performed one of the first electronic-structure calculations of this species. This was a big calculation at the time, done before C_{60} was first synthesized. I also looked at $C_{60}H$ (a paper accepted for publication overnight, my record).

D.S. Marynick, S.K. Estreicher, **Chem. Phys. Lett.** **132**, 383 (1986)

S.K. Estreicher, C.D. Latham, M.I. Heggie, R. Jones, S. Öberg, **Chem. Phys. Lett.** **196**, 311 (1992)

R. Jones, C.D. Latham, M.I. Heggie, V.J.B. Torres, S. Öberg, S.K. Estreicher, **Phil. Mag. Lett.** **65**, 291 (1992)

d) An unusual Jahn-Teller effect: Diatomic molecules in ionic crystals prefer to lie along low-symmetry orientations. It turns out that the high-symmetry ones involve orbital degeneracies which render the molecule Jahn-Teller unstable. Orbital degeneracies are normally lifted by *vibronic* coupling: the electronic orbitals couple to vibrational degrees of freedom and lattice distortions lower the symmetry until the degeneracy is lifted. But here, the degeneracy is lifted by *rotronic* coupling: the electronic orbitals couple to the rotational degrees of freedom of the molecule. The symmetry is lowered as the molecule aligns along lower-symmetry directions: S.K. Estreicher, T.L. Estle, **Phys. Rev. B** **30**, 7 (1984) and **Phys. Rev. B** **31**, 5616 (1985)

e) H-enhanced migration of O: Interstitial O diffuses very slowly in Si, unless traces of H are present in the sample. I proposed the first explanation for this catalytic effect: H stabilizes the saddle point for O diffusion by temporarily saturating a Si dangling bond, causing the migration barrier to drop from ~ 2.6 eV to ~ 1.6 eV:

S.K. Estreicher, Y.K. Park, P.A. Fedders, *Early Stages of Oxygen Precipitation in Si*, ed. R. Jones (Kluwer, 1996), 179.

A question to which I have no answer (if you do, I am interested)

Accelerated charges radiate (e.g., Larmor formula). This in classical and quantum E&M (particle accelerators). Thus an accelerated Si ion or Si nucleus radiates. Now think of N Si nuclei in a crystal. Each nucleus has 3 degrees of freedom. There are $3N-3$ (or $3N-6$ if you insist on rotating the crystal) oscillators. In the zero-point energy state, these oscillating (= continuously accelerated) nuclei cannot radiate or they would lose energy which is impossible because you cannot remove any of the zero-point energy. These are not neutral atoms but charged ions. Some electrons move along, with a little delay. And the same occurs with metals: Cu consists of Cu^+ ions with no bound e^- . We deal here with accelerated charges which do not radiate. The same charges placed between the plates of a capacitor would radiate when accelerated by a constant electric field. But a constant $\underline{E}$ -field means that the potential has no curvature. But as soon as a potential has some curvature, the energy states are quantized and, in the zero-point energy state, the charge is accelerated but cannot radiate. There seems to be something here associated with the curvature of the potential.

Now consider the same Si crystal with some oscillators are in excited states, say zero-point energy plus 3 phonons. The nuclei are accelerated and should radiate, but the oscillator can only lose energy in quanta of $\hbar\omega$. One option is that the nucleus somehow accumulates radiation energy until it equals $\hbar\omega$. And then, the nucleus drops by one vibrational energy level and emits its accumulated radiation energy in a single burst: one photon. But how would such a process of accumulation of radiation energy work? What would be the nature of this energy 'box' that must be filled before its content emerges as one photon? And what makes this process stop when the oscillator reaches the zero-point energy state? There is something weird here, and I don't know how to write an equation for the radiation of accelerated charges that includes both quanta of energy release and a non-radiating zero-point energy state.