2018

2017
S.K. Estreicher, *The beginning of wine and viticulture*  

DOI 10.1002/pssa.201700204

T.M. Gibbons, D.J. Backlund, and S.K. Estreicher, *Cobalt-related defects in silicon*  
*Journal of Applied Physics* 121, 045704/1-6 (2017)

2016
D.J. Backlund, T.M. Gibbons, and S.K. Estreicher, *Vanadium interactions in crystalline silicon*  
*Physical Review B* 94, 195210/1-6 (2016)

*Nature Scientific Reports* 6, 32150/1-10 (2016)  
DOI: 10.1038/srep32150  
http://rdcu.be/pLJe

S.K. Estreicher, T.M. Gibbons, M.B. Bebek, and A. Cardona, *Heat flow and defects in semiconductors: beyond the phonon scattering assumption*  
*Solid State Phenomena* 242, 335-343 (2016)

2015
S.K. Estreicher, *Wine*  


*Journal of Applied Physics* 117, 112801/1-6 (2015)

S. K. Estreicher and A. McDonald (editors), *Proc. 32nd International Conference on the Physics of Semiconductors*  


2014
S.K. Estreicher, *A brief history of wine in South Africa*
European Review 22 (3), 504-537 (2014)

Physical Review B 89, 155409/1-9 (2014)

A. Cavallini and S. K. Estreicher (editors), Proc. 27th International Conference on Defects in Semiconductors,
An Erratum goes with the Preface. How did that happen? JAP 115, 049901 (2014)
American Institute of Physics Proceedings http://scitation.aip.org/content/aip/proceeding/aipcp/1583 (contributed)

S.K. Estreicher, T.M. Gibbons, By. Kang, and M.B. Bebek, Phonons and defects in semiconductors and
nanostructures: phonon trapping, phonon scattering, and heat flow at heterojunctions

S.K. Estreicher, T.M. Gibbons, and M. Stavola, Isotope-dependent phonon trapping at defects in semiconductors

M. Stavola, S.K. Estreicher, and M. Seacrist, Light-element impurities and their reactions in multicrystalline Si

2013

Nickel: a very fast diffuser in Si

T.M. Gibbons, S.K. Estreicher, K. Potter, F. Bekisli, and M. Stavola, Huge isotope effect on the vibrational lifetimes
of an H2*(C) defect in Si
Physical Review B 87, 115207/1-5 (2013)

S.K. Estreicher, A brief history of wine in Spain
European Review 21 (2), 209-239 (2013)

2012

S.K. Estreicher, A. Docaj, M.B. Bebek, D.J. Backlund, and M. Stavola, Hydrogen, H in C-rich Si, and the diffusion of
vacancy-H complexes

S.K. Estreicher, Vibrational dynamics of impurities in semiconductors: phonon trapping and isotope effects
Materials Science Forum 725, 203-208 (2012)

S.K. Estreicher and A. Carvalho, The CuPL defect and the Cu$_{63}$Cu$_{13}$ complex

A. Docaj and S.K. Estreicher, Three carbon pairs in Si

2011

Microscopic structure of a VH$_4$ center trapped by C in Si
Physical Review B 84, 195205/1-7 (2011)
A. Carvalho, D.J. Backlund, and S.K. Estreicher, *Four-copper complexes in Si and the CuPL defect: a first-principles study*


*Physical Review B* **84**, 035317/1-10 (2011), also available in the Max-Planck Society archives

S.K. Estreicher, D.J. Backlund, C. Carbogno, and M. Scheffler, *Activation energies for diffusion of defects in crystalline silicon: The role of the exchange-correlation functional*

*Angewandte Chemie* **50**, 10221-10225 (2011)


**2010**

D.J. Backlund and S.K. Estreicher, *Structural, electrical and vibrational properties of Ti-H and Ni-H complexes in Si*


D.J. Backlund and S.K. Estreicher, *Ti, Fe, Ni in Si and their interactions with the vacancy and the A-center: a theoretical study*


S.K. Estreicher and D.J. Backlund, *Electrically active and electrically inactive 3d transition metal centers in Si*


**2009**


selected for publication in the July 6, 2009 issue of *Virtual Journal of Nanoscale Science & Technology* (AIP/APS)

S.K. Estreicher and T.M. Gibbons, *Non-equilibrium molecular-dynamics for impurities in semiconductors: vibrational lifetimes and thermal conductivities*


S.K. Estreicher, D. Backlund, and T.M. Gibbons, *Non-equilibrium dynamics for impurities in semiconductors*


S.K. Estreicher, D. Backlund, T.M. Gibbons, and A. Doçaj, *Vibrational properties of impurities in semiconductors*

S.K. Estreicher, *Controlling the properties of materials with impurities: What’s new?* Physics @ TTU (Physics Department annual review, Spring 2009)

2008


2007


N. Gonzalez Szwacki and S.K. Estreicher, *First-principles investigations of Fe-H interactions in Si*  

D.J. Backlund and S.K. Estreicher, *Carbon-oxygen interactions in Si*  

M. Sanati and S.K. Estreicher, *Fundamental interactions involving Fe in Si*  

2006


K. K. Kohli, G. Davies, N.Q. Vinh, D. West, S.K. Estreicher, T. Gregorkiewicz, and K.M. Itoh *Isotope dependence of the lifetime of the 1136 cm⁻¹ vibration of oxygen in silicon*  

S.M. Myers, A.F. Wright, M. Sanati, S.K. Estreicher, *Theoretical properties of the N vacancy in p-type GaN(Mg,H) at elevated temperatures*  

D. West and S.K. Estreicher, *First-principles calculations of vibrational lifetimes and decay channels: Hydrogen-related modes in Si*  

This paper was also selected for the April 2006 issue of *Virtual Journal of Ultrafast Science*.

S.K. Estreicher and M. Sanati, *Predicting the energetics of defects at T > 0K*  

S.K. Estreicher and M. Sanati, *Energetics of H and Mu in Semiconductors: theoretical predictions at finite temperatures*  

ISBN: 978-0-87586-476-1 (paper); 978-0-87586-477-8 (hard cover); 978-0-87586-478-5 (ebook)


S.K. Estreicher and D. West, *Vibrational Lifetimes for Light Impurities in Si*  

S.K. Estreicher and M. Stavola, *Hydrogenation Methods and Passivation Mechanisms for c-Si Photovoltaics*  

M. Sanati and S.K. Estreicher, *Oxygen-Boron Complexes in Si*  

A.F. Wright, S.M. Myers, S.K. Estreicher and M. Sanati, *Formation of V₅H and MgV₅H in p-type GaN(Mg,H)*  


**2005**

*Physical Review B* 72, 165206/1-8 (2005)

S.K. Estreicher, D. West, M. Sanati, *'Cu₂': a metastable configuration of the {Cu₆,Cu₆} pair in Si*  
*Physical Review B* 72, 121201(R)/1-4 (2005)

*Physical Review B* 72, 075209/1-6 (2005)

*Physical Review B* 71, 115212/1-7 (2005)

*Solid State Communications* 133, 465-468 (2005)

*Journal of Physics: Condensed Matter* 17, S2211-S2218 (2005)

S.K. Estreicher, *Theory of Defects in Semiconductors: Recent Developments and Challenges*  
*Interfaces* (Spring 2005, guest editor: H. Huff), pp. 28-31

S.K. Estreicher and M. Stavola, *Hydrogenation Methods and Passivation Mechanisms for c-Si Photovoltaics*  

**2004**

S.K. Estreicher, M. Sanati, D. West, and F. Ruymgaart, *Thermodynamics of impurities in semiconductors*  
*Physical Review B* 70, 125209/1-10 (2004)

M. Sanati and S.K. Estreicher, *Specific heat and entropy of GaN*  

M. Sanati, S.K. Estreicher, and M. Cardona, *Isotopic-dependence of the heat capacity of c-C, Si, and Ge: An ab-initio calculation*  
J.L. McAfee, S.K. Estreicher, and He Ren, *Structural and vibrational properties of N, N pairs, and \{N,H\} complexes in Si*


S.K. Estreicher, *First-Principles Theory of Copper in Silicon*
in *Copper interaction with Silicon based materials: a survey*, ed. A. Mesli and O. Aboelfotoh


S.K. Estreicher, *Vibrational Dynamics for Defects in Semiconductors*


M. Sanati and S.K. Estreicher, *Theoretical studies of boron-oxygen complexes in silicon*


D. West, M. Sanati, and S.K. Estreicher, *Temperature-dependence of the dissociation energy of copper pairs in Si*


E.C. Scott, ..., Steven Chu, ..., Stephen W. Hawking, ..., S. Estreicher, ..., Steven Weinberg, ... (443 authors), *The Morphology of Steve*


**2003**

M. Sanati and S.K. Estreicher, *Defects in silicon: the role of vibrational entropy*


M. Sanati and S.K. Estreicher, *First-Principles Thermodynamics for Defects in Silicon*


S.K. Estreicher, *Dynamics of hydrogen in silicon*


S.K. Estreicher, *Defect Theory: an elusive state-of-the-art*


M. Sanati and S.K. Estreicher, *Theory of defects in silicon solar cells at finite temperatures*

13\textsuperscript{th} Wkshp on c-Si Solar Cell Materials and Processes (Vail, CO 8/03), **NREL/BK 520-3443**, 106-109 (2003)
J.L. McAfee and S.K. Estreicher, *Theoretical predictions of complex formation following hydrogenation from a nitride layer*


**2002**


S.K. Estreicher, *The H\textsubscript{2} Molecule in Semiconductors: an Angel in GaAs, a Devil in Si*

S.K. Estreicher, D. West, and P. Ordejón, *Copper-Defect and Copper-Impurity Interactions in Si*

S.K. Estreicher and D. West, *Microscopic Properties of Copper in Si: Theoretical Predictions*

J.L. McAfee and S.K. Estreicher, *Isolated N and N pairs in silicon*
12th Wkshp c-Si Solar Cell Materials and Processes (Breckenridge, CO 8/02), NREL/BK 520-32717, 171-174 (2002)

S.K. Estreicher, D. West, J.M. Pruneda, S. Knack, and J. Weber, *Formation and properties of three copper pairs in silicon*

S.K. Estreicher, *From Fermentation to Transportation: Materials in the History of Wine*

**2001**

Physical Review B 64, 235211/1-7 (2001)

J.E. Lowther, S.K. Estreicher and H. Temkin, *Nitrogen-related complexes in GaAs*

S.K. Estreicher, K. Wells, P.A. Fedders, and P. Ordejón, *Dynamics of hydrogen molecules in Si*

S.K. Estreicher, M. Gharaibeh, P.A. Fedders, and P. Ordejón, *Unexpected dynamics for self-interstitial clusters in silicon*

S.K. Estreicher, P.A. Fedders, and P. Ordejón, *The Fascinating Dynamics of Defects in Silicon*
Physica B 308-310, 1-7 (2001)


2000


1999


B. Hourahine, R. Jones, A.N. Safonov, S. Öberg, P.R. Briddon, and S.K. Estreicher, *Optically active hydrogen dimers in Si*  

S.K. Estreicher, *Copper-related defects in silicon*  


S.K. Estreicher and J.L. Hastings, *Copper-related complexes in silicon*  

1998

S.K. Estreicher, J.L. Hastings, and P.A. Fedders, *Defect-induced dissociation of H₂ in silicon*  

M. Stavola and S.K. Estreicher, *Recent Experimental and Theoretical Results for H₂ in Silicon*  


S.K. Estreicher, *The Wines from Porto*  
*Lubbock Magazine, June 1998*, p.8-12


1997

J.L. Hastings, S.K. Estreicher, and P.A. Fedders, *Vacancy aggregates in silicon*  


S.K. Estreicher and P.A. Fedders, *Molecular-dynamics simulations of microscopic defects in Si*  

S.K. Estreicher and P.A. Fedders, *Molecular-dynamics modeling of hydrogen in silicon*  

S.K. Estreicher and D.E. Boucher, *Theoretical studies in GaN*, in  

J.L. Hastings, S.K. Estreicher, and P.A. Fedders, *Vacancy aggregates in silicon*  


1996

Solar Energy Materials and Solar Cells **41/42**, 159-169 (1996)


S.K. Estreicher and Dj.M. Maric, *Theoretical study of hydrogen in cubic GaN*  


1995


S.K. Estreicher, *Hydrogen in wide bandgap semiconductors*  

S.K. Estreicher, *Hydrogen-related defects in crystalline semiconductors: A theorist's perspective*  


1994
S.K. Estreicher, M.A. Roberson, Dj.M. Maric, *Hydrogen and H dimers in c-C, Si, Ge, and α-Sn*

M.A. Roberson and S.K. Estreicher, *Vacancy and vacancy-hydrogen complexes in silicon*

S.K. Estreicher and R. Jones, \( \{H,P\}^0 \rightarrow \{H,P\}^+ \) transitions: A new look at donor-H pairs in Si

S.K. Estreicher, *Hydrogen in semiconductors: The roles of µSR and theory*


S.K. Estreicher and R. Jones, *Passivation and reactivation of \{H,P\} pairs in Si*


Dj.M. Maric, M.A. Roberson, S.K. Estreicher, *Relative stability of \( H_1 \) vs. \( H_1^+ \) and \( H_2 \) vs. \( H_2^+ \) in c-C, Si, Ge, α-Sn and consequences*

*Cross Cuts* **3/2**, 1 and 4-6 (1994)

1993

S.K. Estreicher and Dj.M. Maric, *What is so strange about hydrogen interactions in Ge?*

Dj.M. Maric, P.F. Meier, and S.K. Estreicher, *\{H,B\}, \{H,C\}, and \{H,Si\} pairs in Si and Ge*

S.K. Estreicher, Dj.M. Maric, P.F. Meier, and D.S. Marynick, *Very large scale electronic structure calculations with PRDDO*
*Cross Cuts* **2/3**, 5-6 (1993)

1992
L. Korpas, J.W. Corbett, S.K. Estreicher, *Multiple trapping of H at boron and phosphorus in Si*


S.K. Estreicher, *Theoretical studies of defects, impurities, and complexes in semiconductors*


M.A. Roberson and S.K. Estreicher, *Interstitial impurities in wurtzite vs. zincblende semiconductors: The case of H in SiC*


1991

M.A. Roberson and S.K. Estreicher, *Interstitial hydrogen in cubic and hexagonal SiC*


1990


S.K. Estreicher, *Interstitial O in Si and its interactions with H*  

S.K. Estreicher, *Copper, lithium, and hydrogen passivation of boron in c-Si*  
Physical Review B 41 (rapid communication), 5447-5450 (1990)

Hyperfine Interactions 64, 573-578 (1990)

1989


S.K. Estreicher, L. Throckmorton and D.S. Marynick, *Hydrogen passivation of shallow acceptors and donors in c-Si: comparisons and trends*  

1988

S.K. Estreicher, *Surface and size effects for impurities in Si clusters*  
Physical Review B 37, 858-863 (1988)

1987

S.K. Estreicher, *Equilibrium sites and electronic structure of interstitial hydrogen in Si*  

T.L. Estle, S.K. Estreicher, and D.S. Marynick, *Bond-centered H or Mu in diamond: The explanation for Mu* and an example of metastability*  
Physical Review Letters 58, 1547-1550 (1987)

1986


D.S. Marynick and S.K. Estreicher, *Localized molecular orbitals and electronic structure of C_60*  
T.L. Estle, S.K. Estreicher and D.S. Marynick, Preliminary calculations confirming that anomalous muonium is bond-centered interstitial muonium

S.K. Estreicher and D.S. Marynick, Lattice relaxation for normal muonium in diamond
_Hyperfine Interactions_ **32**, 613-617 (1986)

**1985**
S.K. Estreicher, A.K. Ray, J.L. Fry and D.S. Marynick, Surface effects in cluster calculations of energy profiles of Mu in diamond,

S.K. Estreicher and T.L. Estle, Mechanisms for orthorhombic Jahn-Teller distortions of orbital triplets

**1984**
S.K. Estreicher and T.L. Estle, Rotronic Jahn-Teller effect for diatomic molecules in ionic crystals

S.K. Estreicher and P.F. Meier, Change of energy profiles for muons upon lattice relaxation

S.K. Estreicher, P.F. Meier, Influence of lattice relaxation and zero-point motion on hyperfine fields at muons in ferromagnetic metals

S.K. Estreicher and P.F. Meier, Trapping of muons in doped Al and Cu

**1983**
S.K. Estreicher and P.F. Meier, Energy profiles for light impurities in simple metals

S.K. Estreicher and P.F. Meier, Parameterization of the self-consistently calculated charge density around a proton in jellium

**1982**
S.K. Estreicher and P.F. Meier, Hyperfine fields at impurities in ferromagnetic metals

S.K. Estreicher, Light impurities in simple metals: electronic structure and energy profiles
_PhD dissertation_, University of Zürich (1982)

**1981**
_Hyperfine Interactions_ **9**, 611-616 (1981)

S.K. Estreicher and P.F. Meier, Effects of the zero-point motion on the hyperfine field at the muon