

SANDIA REPORT

SAND2012-3313

Unlimited Release

Printed April 2012

Simple intrinsic defects in InP: Numerical predictions

Peter A. Schultz

Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Approved for public release; further dissemination unlimited.



Sandia National Laboratories

Issued by Sandia National Laboratories, operated for the United States Department of Energy by Sandia Corporation.

NOTICE: This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government, nor any agency thereof, nor any of their employees, nor any of their contractors, subcontractors, or their employees, make any warranty, express or implied, or assume any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represent that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government, any agency thereof, or any of their contractors or subcontractors. The views and opinions expressed herein do not necessarily state or reflect those of the United States Government, any agency thereof, or any of their contractors.

Printed in the United States of America. This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831

Telephone: (865) 576-8401
Facsimile: (865) 576-5728
E-Mail: reports@adonis.osti.gov
Online ordering: <http://www.osti.gov/bridge>

Available to the public from
U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Rd.
Springfield, VA 22161

Telephone: (800) 553-6847
Facsimile: (703) 605-6900
E-Mail: orders@ntis.fedworld.gov
Online order: <http://www.ntis.gov/help/ordermethods.asp?loc=7-4-0#online>



SAND2012-3313
Unlimited Release
Printed April 2012

Simple intrinsic defects in InP: Numerical predictions

Peter A. Schultz
Advanced Device Technologies, Dept. 1425
Sandia National Laboratories
P.O. Box 5800
Albuquerque, New Mexico 87185-MS1322

Abstract

This Report presents numerical tables summarizing properties of intrinsic defects in indium phosphide, InP, as computed by density functional theory, intended for use as reference tables for a defect physics package in device models, and for use as part of training sets in developing interatomic potentials for InP.

This page intentionally left blank

CONTENTS

Simple intrinsic defects in InP: Numerical predictions	3
1. Introduction.....	7
1.1. Computational methods	7
1.2. Verification and validation	7
1.2.1. Extrapolation model	9
1.2.2. Verification and validation of InP defect results.....	10
2. Results.....	11
2.1. Defect atomic structures	11
2.2. Defect charge transition energy levels.....	12
2.3. Defect formation energies.....	15
2.4. Defect migration energies	16
2.4.1. Indium interstitial – thermal diffusion.....	16
2.4.2. Phosphorus interstitial – thermal diffusion	17
2.4.3. Athermal and recombination enhanced diffusion	17
2.5. Neutral defect formation energies.....	17
3. Conclusions.....	19
4. References.....	19
Appendix A: Neutral defect atomic configurations.....	21

TABLES

Table 1. Computed bulk InP properties	8
Table 2. Supercell extrapolation energies, $\epsilon_0=12.5$, $R_{\text{skin}}=1.6$ bohr.....	10
Table 3. Ground state structure designations for vacancy and antisite defects.	11
Table 4. Ground state structure designations for the interstitials and di-antisite.....	11
Table 5. Defect levels for the indium vacancy, in eV, referenced to the VBE: $v_{\text{In}} (v') \leftrightarrow v_{\text{P}}\text{-P}_{\text{In}} (v^*)$	12
Table 6. Defect levels for the phosphorus vacancy, in eV, referenced to the VBE: $v_{\text{P}} (v') \leftrightarrow v_{\text{In}}\text{-In}_{\text{P}} (v^*)$	12
Table 7. Defect levels for the divacancy, in eV, referenced to the VBE: $v_{\text{V}} = v_{\text{P}}\text{---}v_{\text{In}}$	13
Table 8. Defect levels for the phosphorus antisite, in eV, referenced to the VBE: $a_{\text{P}} = \text{P}_{\text{In}}$	13
Table 9. Defect levels for the indium antisite, in eV, referenced to the VBE: $a_{\text{In}} = \text{In}_{\text{P}}$	13
Table 10. Defect levels for the di-antisite, in eV, referenced to the VBE: $aa = \text{In}_{\text{P}}\text{---}\text{P}_{\text{In}}$	14
Table 11. Defect levels for the indium interstitial, in eV, referenced to the VBE: $i_{\text{In}} = \text{In}_i$	14
Table 12. Defect levels for the phosphorus interstitial, in eV, referenced to the VBE: $i_{\text{P}} = \text{P}_i$	14
Table 13. Formation energies of InP defects at VBE, in eV, context = LDA.	15
Table 14. Formation energies of InP defects at VBE, in eV, context = LDA-3d.....	15
Table 15. Formation energies of InP defects at VBE, in eV, context = PBE.	16
Table 16. Diffusion barriers (thermal) for the indium interstitial, in eV.	16
Table 17. Diffusion barriers (thermal) for the phosphorus interstitial, in eV.	17
Table 18. Formation energies of neutral defects for InP (in eV).	18

NOMENCLATURE

CBE	conduction band edge
DFT	density functional theory
eV	electron Volt
FDSM	finite defect supercell model
GGA	generalized gradient approximation
IP	ionization potential
LDA	local density approximation
LMCC	local moment countercharge
MSMSE	Modelling and Simulation in Materials Science and Engineering
n/c	not computed
n/x	not exist
PAS09	Article: P.A. Schultz and O.A. von Lilienfeld, MSMSE 17 , 084007 (2009).
PBE	Perdew/Burke/Ernzerhof, a “flavor” of GGA
PP	pseudopotential
SNL	Sandia National Laboratories
TS	transition state
VBE	valence band edge

1. INTRODUCTION

The numerical results for density functional theory (DFT) calculations of properties of simple intrinsic defects in indium phosphide are presented. The results of the defect calculations are summarized into a series of numerical Tables containing the parameters needed to populate defect physics packages needed for device simulations. In addition, a summary of the InP-specific verification and validation evidence is presented that provides a basis for estimating an overall uncertainty in predicted defect energy levels of the same size as for earlier simulations of silicon defects [1] and GaAs defects [2] (henceforth, “PAS09”), namely, 0.1-0.2 eV accuracy/uncertainty.

1.1. Computational methods

The details of the computational methods are comprehensive described previously in PAS09 (as applied to GaAs), and will only be briefly summarized here. The DFT calculations were performed with the SEQQUEST code. [3] The defect calculations were performed using both the local density approximation (LDA) [4] and the Perdew-Burke-Ernzerhof (PBE) flavor of the generalized gradient approximation [5], this comparison being a partial assessment of the physical uncertainties within DFT functionals [6]. Calculations with both $3d$ -core and $3d$ -valence pseudopotentials (PP) were used for the indium atom, to test (verify) the convergence in the PP construction for defect properties.

The calculations of charged defects used the Finite Defect Supercell Model (FDSM) [1] to incorporate rigorous boundary conditions for the solution of the electrostatic potential in a charged supercell [7] and extrapolate the computed defect energies to the infinitely dilute limit. Defect calculations were performed using 64-atom, 216-atom, and 512-atom cubic supercells. The 216-site supercell calculations proved to be sufficiently converged to achieve the required accuracy and are the default production calculations listed in this Report.

These simulation contexts are labeled in the following as: LDA64, LDA, and LDA512, for 64-site, 216-site, and 512-site, respectively, supercell calculations using LDA and the $3d$ -core ($Z=3$) PP for In; PBE for the 216-site supercells using PBE and $3d$ -core PP; and LDA-3d and PBE-3d for the 216-site supercells with $3d$ -valence ($Z=13$) PP for the In atoms.

1.2. Verification and validation

The defect level calculations all used SEQQUEST and the FDSM, the same methods used in DFT calculations of defects in silicon and GaAs, which yielded mean absolute errors of 0.1 eV and maximum absolute error of 0.2 eV for defect levels over a wide sampling of different defects. This is the expected accuracy (uncertainties) of the methods for these defect level calculations in InP, and the limit of the physical accuracy of the DFT approximations used in this analysis.

The phosphorus PP has been described previously [8], and are the same used in the silicon defect calculations [1]: a standard s^2p^3 valence atom, added a d -potential with $R_c=1.08$ Bohr to use as the local potential. The indium PP was developed using the same systematic procedure used for the gallium PP for GaAs [8]. Both the $3d$ -core and $3d$ -valence PP were constructed within the generalized norm-conserving pseudopotential method of Hamann [9]. The $3d$ -core In PP was extended to use a “hard” f -potential ($R_f=1.1$ Bohr) as the local potential and also added a partial core correction [10] to enhance transferability. The d -potential of the $3d$ -valence potential did not

require a partial core correction and using the d -potential as the local potential achieves good transferability.

The In potentials all gave a good description of the experimental body-centered-tetragonal ground state structure of bulk In, preferring the bct (body-centered-tetragonal) structure over a fcc (face-centered-cubic) structure. For the P atom, the defect formation energy calculations use the optimum A7 structure as the reference structure: to maintain commonality with the GaAs calculations, and also to avoid a known shortcoming of DFT in describing the experimental A17 structure ground structure (differential van der Waals binding) that would bias the comparison between the LDA and PBE results for InP defects.

As a test of transferability, all the LDA calculations were performed with both the $3d$ -core and $3d$ -valence PP for In. While absolute formation energies (of neutral defects) differed by as much as 0.26 eV (for the indium antisite, In_P), the differences were typically much smaller. The largest difference between computed defect level between the $3d$ -core and $3d$ -valence PP was 0.08 eV, and the average deviation was less than 0.02 eV (over half of the computed levels are within 0.01 eV), indicating an effective cancellation of errors was occurring. Hence, uncertainties in the absolute formation energies might be as large as 0.26 eV, but the ($3d$ -core) defect levels, obtained as differences in formation energies, have much smaller uncertainties, less than 0.1 eV, with respect to pseudopotential construction. The bulk properties obtained for InP with these simulation contexts are in the following Table.

Table 1. Computed bulk InP properties

Simulation context	Lattice parameter (Å)	Bulk Modulus (GPa)	Kohn-Sham Band gap (eV)	Formation energy (eV)
Experiment	5.866 (a)	72.5 (b)	1.42 (c)	0.50 (d)
LDA	5.854	68.4	0.67	0.383
LDA-3d	5.844	71.8	0.66	0.179
PBE	5.983	57.7	0.47	0.516
PBE-3d	5.975	58.9	0.46	0.568

- (a) Ref. [11].
- (b) Ref. [12].
- (c) Ref. [13].
- (d) Ref. [14].

Comparisons of experimental formation energies to computed formation energies are problematic for phosphides, both because DFT has difficulties with the van der Waals part of the bonding in some bulk phosphorus allotropes, and because experimental assessments are also complicated by the uncertainties in relative formation energies of different phosphorus allotropes [14]. The listed values, experimental and theoretical, use black phosphorus as the elemental reference (although the experiment uses the A17 structure and the DFT the A7 structure). The apparent good agreement between experiment and the simulations should be regarded skeptically and as somewhat fortuitous.

Comparison of InP defect results with different functionals, LDA vs. PBE, provides an indication of the size of the uncertainty due to the DFT physical approximation. While mostly very similar, the numerical differences in LDA and PBE computed defect levels are as large as 0.3 eV. Results for silicon defects indicated that PBE values are more reliable (lower maximum errors) for $-U$ transitions involving structural rearrangements. The InP defects are predicted to have multiple $-U$ transitions and structural rearrangements, suggesting PBE might be necessary to achieve the 0.1-0.2 eV target accuracy seen in computations of defect levels in silicon and GaAs.

1.2.1. Extrapolation model

The total energy calculations for the charged defects used a modified-Jost model [15, 1] to evaluate the missing charge polarization (screening) energy outside the finite volume of the supercell:

$$E_{\text{pol}} = (1 - 1/\epsilon_0) q^2/R_{\text{Jost}} \quad (1)$$

where ϵ_0 is the static dielectric constant, and $R_{\text{Jost}} = (R_{\text{sphere}} - R_{\text{skin}})$ is the radius of a sphere with a volume equal to the volume of the supercell, R_{sphere} , less the skin depth, R_{skin} , of an unscreened surface region within the sphere. R_{skin} must be calibrated (fit) once for each material system.

The *extrapolation model* was *calibrated* via calculations of negative charge states of the indium vacancy, in unrelaxed tetrahedral structures for the (1-), (2-), and (3-) charge states.

The *extrapolation model* was then *verified* using the (0/1+) and (1+/2+) transitions of the P_{In} antisite and also the As_{In} iso-antisite defect, via comparisons of defect levels extrapolated to infinitely dilute defects from 64-site, from 216-site, and from 512-site supercell calculations. 216-site cells were assessed to be necessary to meet required level of quantitative confidence. The $\nu\nu$ divacancy (as an example of a low-symmetry defect expected to have large spatial extent) with 216-site supercells was repeated using 512-site supercells as a further verification test. The differences in any defect level was typically smaller than 0.05 eV, indicating uncertainty with respect to cell size (and k-point sampling) is less than 0.05 eV, even for the extreme charge states (of the $\nu\nu$).

The *extrapolation model* was *validated*. The experimental InP dielectric constant, 12.5 [16], for ϵ_0 and a physically reasonable unpolarized “skin depth” (R_{skin}), 1.6 bohr, led to a converged extrapolation, and these parameters are also consistent with extrapolation models in multiple other III-V defect calculations such as GaAs, AlAs, and GaP (experimental ϵ_0 and $R_{\text{skin}}=1.5(2)$)

The quantities defining the extrapolation model are summarized in the following Table.

Table 2. Supercell extrapolation energies, $\epsilon_0=12.5$, $R_{\text{skin}}=1.6$ bohr.

Context:	LDA64	LDA512	LDA	LDA-3d	PBE	PBE-3d
$a_0(\text{\AA})$	5.854	5.854	5.854	5.844	5.983	5.975
IP(VBE) (eV)	5.15	5.33	5.23	5.20	5.16	n/c
Charge	External polarization energy (eV), Eq. 1					
$ q = 1$	1.0324	0.4842	0.6593	0.6605	0.6439	0.6447
$ q = 2$	4.1296	1.9370	2.6370	2.6420	2.5757	2.5789
$ q = 3$	9.,2915	4.3582	5.9333	5.9444	5.7953	5.8025
$ q = 4$	16.5182	7.7479	10.5482	10.5678	10.3028	10.3156

1.2.2. Verification and validation of InP defect results

There is little experimental data available to quantitatively validate InP defect level results. The phosphorus antisite is believed to exist, but its levels are variously described as just above and just below the conduction band edge, or mid-gap and 0.5 eV below the conduction band edge. There is no certainty in any other defect identification of a primal defect. There is a need to acquire good data, both for validation of the theoretical results, but even to calibrate the position of the band edges on the computed defect level diagram.

Previous simulations of InP are not immediately useful for (“weak”) verification. In addition to there not being many previous simulations, of relatively recent and converged results, comparisons of even neutral formation energies, not subject to differences in charge supercell treatments, are also problematic, and for the same reason that comparisons to the experimental formation energy of bulk InP were: the elemental reference of phosphorus is inadequately specified to construct meaningful quantitative comparisons. This further highlights to need for greater, more precise experimental data for defects in InP.

2. RESULTS

The section contains the Tables that summarize the numerical results for DFT simulations of defects in InP.

2.1. Defect atomic structures

The following Tables list ground state structures for simple intrinsic defects in InP as a function of charge state. Bonding structures are illustrated (for GaAs) in PAS09. For the vacancies, v' refers to the simple vacancy, and v^* refers to the site-shifted form of the vacancy (where a nearest-atom to the vacancy hops into the vacant site, thus creating a vacancy-antisite pair).

Table 3. Ground state structure designations for vacancy and antisite defects.

Charge state	$v' = v_{\text{In}} \leftrightarrow v^* = v_{\text{P}}\text{In}$	$v' = v_{\text{P}} \leftrightarrow v^* = v_{\text{In}}\text{InP}$	vv	$a\text{P}$	$a\text{In}$
(4-)	-	-	$C_{1h}\text{-pair}(\text{In})$	-	-
(3-)	v'/T_d	$v'/\text{res-}D_{2d}$	$C_{1h}\text{-pair}(\text{In})$	-	-
(2-)	$v'/\sim T_d$	$v'/\text{pair-}D_{2d}$	$C_{3v}\text{-in}(\text{In}) \{\text{lda}\}$ $C_{1h}\text{-pair}(\text{In}) \{\text{lda-3d, pbe}\}$	$*C_{3v}$	T_d
(1-)	$v^*/C_{1h}\text{-pair}(\text{In})$	$v'/\text{pair-}D_{2d}$	$C_{3v}\text{-in}(\text{In})$ $C_{1h}\text{-pair}(\text{In}) \{\text{pbe}\}$	$*C_{3v}$	$\text{res-}D_{2d}$
(0)	$v^*/C_{1h}\text{-pair}(\text{In})$	$v'/\text{pair-}D_{2d}$	$C_{3v}\text{-out}(\text{In})$	T_d	$\text{res-}D_{2d}$
(1+)	$v^*/C_{3v}\text{-in}(\text{In})$ $v^*/C_{1h}\text{-pair}(\text{In}) \{\text{pbe}\}$	$v'/\text{pair-}C_{2v}$	$\sim C_{3v}\text{-out}(\text{In})$	T_d	$\text{res-}D_{2d}$
(2+)	$v_{\text{be}} \{\text{lda, lda-3d}\}$ $v^*/C_{3v}\text{-out}\{\text{pbe3d}\}$	$v'/T_d\text{-out}(\text{In})$	$\sim C_{3v}\text{-out}(\text{In})$	T_d	$\text{pair-}D_{2d}$
(3+)	$v^*/C_{3v}\text{-out}(\text{In})$	$v'/T_d\text{-out}(\text{In})$	-	-	T_d
(4+)	-	-	-	-	T_d

Table 4. Ground state structure designations for the interstitials and di-antisite.

Charge state	In_i	P_i	$aa^{(a)}$ (C_{3v})
(2-)	-	-	C_{3v}
(1-)	$C_{2v}\text{ split-}(110)_{\text{In}}$	$C_2\text{-twisted split-}110_{\text{P}}$	C_{3v}
(0)	$C_{2v}\text{ split-}(110)_{\text{In}}$	$^{(b)}C_{2v}\text{ split-}110_{\text{P}}$ $C_2\text{-twisted split-}110_{\text{P}} \{\text{pbe}\}$	C_{3v}
(1+)	$T_{i,\text{In}} \{\text{lda}\}$ $T_{i,\text{P}} \{\text{lda-3d, pbe}\}$	$C_{1h}\text{ p-}(001)_{\text{In}}$	C_{3v}
(2+)	$T_{i,\text{P}}$	$C_{3v}\text{ H-site}$	C_{3v}
(3+)	$T_{i,\text{P}}$	$T_{i,\text{P}}$	C_{3v}
(4+)	-	-	C_{3v}

(a) Symmetry-reducing distortions (to C_{1h}) yield negligible energy lowering.

(b) The $C_2\text{-twisted split-}110_{\text{P}}$ is only 2 meV higher for LDA contexts (8 meV lower for PBE).

2.2. Defect charge transition energy levels

This section presents the defect charge transition levels of the simple intrinsic defects in InP, in eV, along with neutral defect formation energies. The defect level calculations are the primary result of the Report, the later formation energies are all derived from these results.

Table 5. Defect levels for the indium vacancy, in eV, referenced to the VBE: $v_{In}(v') \leftrightarrow v_{P-P_{In}}(v^*)$

V_{In} Context	Neutral formation energy	Defect levels (eV), cf. VBE						
		(3+/2+)	(2+/1+)	(1+/0)	(0/1-)	(1-/2-)	(2-/3-)	(3-/4-)
Unrelaxed T_d-v' (for polarization calibration)								
LDA64	3.167	n/c	n/c	n/c	0.573	0.922	1.320	n/x
LDA	3.244	n/c	n/c	n/c	0.618	0.946	1.344	n/x
LDA512	3.327	n/c	n/c	n/c	0.606	0.934	1.331	n/x
Relaxed thermodynamic levels								
LDA	3.00	0.33	0.10	1.14	1.23	0.88	0.84	n/x
LDA-3d	3.06	0.32	0.12	1.16	1.24	0.76	0.84	n/x
PBE	2.81	0.64	0.11	1.16	1.24	0.86	0.81	n/x
PBE-3d	n/c	n/c	n/c	n/c	n/c	n/c	n/c	-

Table 6. Defect levels for the phosphorus vacancy, in eV, referenced to the VBE: $v_P(v') \leftrightarrow v_{In-In_P}(v^*)$

V_P Context	Neutral formation energy	Defect levels (eV), cf. VBE						
		(3+/2+)	(2+/1+)	(1+/0)	(0/1-)	(1-/2-)	(2-/3-)	(3-/4-)
LDA	2.68	0.35	-0.13	1.01	0.78	1.65	1.57	n/x
LDA-3d	2.73	0.36	-0.13	1.02	0.80	1.66	1.57	n/x
PBE	2.72	0.51	0.04	1.10	0.85	1.56	1.61	n/x
PBE-3d	n/c	n/c	n/c	n/c	n/c	n/c	n/c	-

Table 7. Defect levels for the divacancy, in eV, referenced to the VBE: $vV = v_P - v_{In}$

Context	Neutral formation energy	Defect levels (eV), cf. VBE						
		(3+/2+)	(2+/1+)	(1+/0)	(0/1-)	(1-/2-)	(2-/3-)	(3-/4-)
LDA512	4.35	n/x	0.20	0.32	0.81	0.60	1.66	1.77
LDA	4.33	n/x	0.16	0.31	0.84	0.60	1.65	1.77
LDA-3d	4.33	n/x	0.18	0.33	0.84	0.61	1.65	1.78
PBE	3.80	n/x	0.13	0.29	1.16	0.58	1.64	1.74
PBE-3d	n/c	-	n/c	n/c	n/c	n/c	n/c	n/c

Table 8. Defect levels for the phosphorus antisite, in eV, referenced to the VBE: $aP = P_{In}$

Context	Neutral formation energy	Defect level (eV), cf. VBE						
		(3+/2+)	(2+/1+)	(1+/0)	(0/1-)	(1-/2-)	(2-/3-)	(3-/4-)
LDA64	1.958	n/x	0.859	0.961	n/x			
LDA512	1.953	n/x	0.848	0.959	n/x			
LDA	1.950	n/x	0.850	0.963	-	-		
LDA-3d	1.95	n/x	0.86	0.96	-	-		
PBE	1.66	n/x	0.82	0.89	n/x			
PBE-3d	n/c	-	n/c	n/c	-			

Table 9. Defect levels for the indium antisite, in eV, referenced to the VBE: $aln = In_P$

Context	Neutral formation energy	Defect level (eV), cf. VBE						
		(4+/3+)	(3+/2+)	(2+/1+)	(1+/0)	(0/1-)	(1-/2-)	(2-/3-)
LDA	2.81	-0.11	0.05	0.36	0.50	0.89	1.09	n/x
LDA-3d	3.07	-0.05	0.10	0.42	0.56	0.97	1.17	n/x
PBE	3.13	-0.04	0.09	0.39	0.52	0.91	1.10	n/x
PBE-3d	n/c	-	-	n/c	n/c	n/c	n/c	-

Table 10. Defect levels for the di-antisite, in eV, referenced to the VBE: $aa = \text{In}_P - \text{P}_{\text{In}}$

aa (C_{3v}) Context	Neutral formation energy	Defect levels (eV), cf. VBE						
		(4+/3+)	(3+/2+)	(2+/1+)	(1+/0)	(0/1-)	(1-/2-)	(2-/3-)
LDA512	2.53	-0.01	0.12	0.29	0.54	1.45	1.51	n/x
LDA	2.54	-0.07	0.09	0.35	0.57	1.47	1.50	n/x
LDA-3d	2.80	-0.03	0.13	0.40	0.62	1.47	1.48	n/x
PBE	2.71	-0.01	0.14	0.39	0.61	1.39	1.43	n/x
PBE-3d	n/c	n/c	n/c	n/c	n/c	n/c	n/c	n/c

Table 11. Defect levels for the indium interstitial, in eV, referenced to the VBE: $\text{In}_i = \text{In}_i$

In_i Context	Neutral formation energy	Defect levels (eV), cf. VBE						
		(3+/2+)	(2+/1+) ^(b) ($T_{i,P}[+]$)	(1+/0) ^(b) ($T_{i,P}[+]$)	(0/1-)	(3+/2+)	(2+/1+) ^(c) ($T_{i,\text{In}}[+]$)	(1+/0) ^(c) ($T_{i,\text{In}}[+]$)
LDA	4.11	0.43	0.62	1.81	1.32	0.43	0.57	1.85
LDA-3d	4.19	0.43	0.61	1.83	1.32	-	-	-
PBE	4.21	0.48	0.64	1.81	1.27	-	-	-
PBE-3d	n/c	n/c	n/c	n/c	n/c	n/c	n/c	n/c

(a) Thermodynamic levels traversing charge state ground states: $T_{i,P}(1+) - T_{i,P}(2+) - T_{i,P}(3+)$.

(b) For LDA context, $\text{In}_i(1+)$ ground state is $T_{i,\text{In}}$ site.

**Table 12. Defect levels for the phosphorus interstitial, in eV, referenced to the VBE:
 $iP = P_i$**

P_i Context	Neutral formation energy	Defect levels (eV), cf. VBE						
		(3+/2+)	(2+/1+)	(1+/0)	(0/1-)	(1-/2-)	(2-/3-)	(3-/4-)
LDA	3.12	0.49	0.07	1.14	1.05	n/x		
LDA-3d	3.11	0.47	0.08	1.11	1.05	n/x		
PBE	2.94	0.53	-0.01	1.17	1.06	n/x		
PBE-3d	n/c	n/c	n/c	n/c	n/c	-		

2.3. Defect formation energies

The ground state defect formation energies, as a function of charge state are trivially obtained by simple arithmetic from the neutral formation energies and the computed defect charge transition energy levels in the previous section. The defect formation energies in these Tables are presented in the phosphorus-rich (A7-structure) limit. The formation energies of the charged defects are presented with the Fermi level at the VBE. The Tables present the formation energies of all the simple intrinsic defects, segregated by simulation context.

The indium interstitial for the LDA context quotes two formation energies for the (1+) charge. The first value is the ground state of the (1+) state in the non-bond tetrahedral interstitial site with P nearest neighbors, $T_{i,P}$, the ground state in all the other contexts, while the second value quotes the formation energy for the $T_{i,In}$.

Table 13. Formation energies of InP defects at VBE, in eV, context = LDA.

Charge state	vIn	vP	vv	aP	aln	aa	iln $T_{i,P}; T_{i,In}$	iP
(4-)	-	-	9.19	-	-	-	-	-
(3-)	5.95	6.68	7.42	-	-	-	-	-
(2-)	5.11	5.11	5.77	-	4.79	5.51	-	-
(1-)	4.23	3.46	5.17	-	3.70	4.01	5.43	4.17
(0)	3.00	2.68	4.33	1.95	2.81	2.54	4.11	3.12
(1+)	1.86	1.67	4.02	0.99	2.31	1.97	2.30;2.26	1.98
(2+)	1.76	1.80	3.86	0.14	1.95	1.62	1.68	1.91
(3+)	1.43	1.45	-	-	1.90	1.53	1.25	1.42
(4+)	-	-	-	-	2.01	1.60	-	-

Table 14. Formation energies of InP defects at VBE, in eV, context = LDA-3d.

Charge state	vIn	vP	vv	aP	aln	aa	iln	iP
(4-)	-	-	9.21	-	-	-	-	-
(3-)	5.90	6.76	7.43	-	-	-	-	-
(2-)	5.06	5.19	5.78	-	5.21	5.75	-	-
(1-)	4.30	3.53	5.17	-	4.04	4.27	5.51	4.16
(0)	3.06	2.73	4.33	1.95	3.07	2.80	4.19	3.11
(1+)	1.90	1.71	4.00	0.99	2.51	2.18	2.36	2.00
(2+)	1.78	1.84	3.82	0.13	2.09	1.78	1.75	1.92
(3+)	1.46	1.48	-	-	1.99	1.65	1.32	1.45
(4+)	-	-	-	-	2.04	1.68	-	-

Table 15. Formation energies of InP defects at VBE, in eV, context = PBE.

Charge state	vIn	vP	vv	aP	aln	aa	iln	iP
(4-)	-	-	8.92	-	-	-	-	-
(3-)	5.72	6.74	7.18	-	-	-	-	-
(2-)	4.91	5.13	5.54	-	5.14	5.53	-	-
(1-)	4.05	3.57	4.96	-	4.04	4.10	5.48	4.00
(0)	2.81	2.72	3.80	1.66	3.13	2.71	4.21	2.94
(1+)	1.65	1.62	3.51	0.77	2.61	2.10	2.40	1.77
(2+)	1.54	1.58	3.38	-0.05	2.22	1.71	1.76	1.78
(3+)	0.90	1.07	-	-	2.13	1.57	1.28	1.25
(4+)	-	-	-	-	2.17	1.58	-	-

2.4. Defect migration energies

Only two intrinsic defects are potentially mobile: the In_i and P_i . All other defects are likely immobile at room or operating temperature (certainly for the time scales of interest for radiation damage). The phosphorus interstitial is not predicted to undergo athermal diffusion [17]. In addition to potential thermal diffusion in *p*-type, both P_i the In_i *might* exhibit recombination-enhanced diffusion (via carrier-driven Bourgoin-Corbett diffusion [18]) in *n*-type InP.

2.4.1. Indium interstitial – thermal diffusion

The In interstitial can take charge states ranging from (1-) to (3+) charge states, according to the results of the DFT calculations. The non-bonded tetrahedral interstitial positions are strongly favored for positively charged, and the bonding (into the network) positions are favored otherwise. The positively charged indium interstitial can potentially migrate thermally, through either the hexagonal site (via a $T_{i,P}-H-T_{i,In}-H-T_{i,P}$ path) or through a split-(110)_{In} site (via a kick-out mechanism) with structural barriers near 1 eV. In *n*-type, the presence of multiple, low energy competitive structures suggest thermal and perhaps recombination enhanced diffusion is possible for In_i .

Table 16. Diffusion barriers (thermal) for the indium interstitial, in eV.

Pathway:	Hexagonal site (<i>H</i>)			Split-(110) _{In} site		
	$\text{In}_i(1+)$	$\text{In}_i(2+)$	$\text{In}_i(3+)$	$\text{In}_i(1+)$	$\text{In}_i(2+)$	$\text{In}_i(3+)$
Context						
LDA	1.00	0.89	0.85	0.72	0.83	1.05
LDA-3d	1.02	0.93	0.86	0.70	0.84	1.04
PBE	0.94	0.87	0.88	0.70	0.83	1.04
PBE-3d	n/c	n/c	n/c	n/c	n/c	n/c

2.4.2. Phosphorus interstitial – thermal diffusion

Unlike in GaAs, no fully connected diffusion path emerged from the ground state search that would lead to net migration. Along the non-bonded $T_{i,P}—H—T_{i,In}$ pathway, the T site is a local maximum, and higher than the H site: the hexagonal (H) site is not a saddle point between the lower-energy T sites. The barrier through the $T_{i,In}$ site is bounded above by the local maximum, and likely much less as a pathway goes around it. Specific H to H' pathways would need to be investigated to determine the minimum energy pathway and associated diffusion barrier. The large number of low-energy (<1 eV) competitive structures for many charge states (along with frequent changes in ground state structure with changes in charge state) suggest the possibility of thermal diffusion in n -type InP.

Table 17. Diffusion barriers (thermal) for the phosphorus interstitial, in eV.

Context	P _i (2+) <1.0eV				P _i (3+) <1.0 eV		
	110 _p	T _{i,P}	H	T _{i,In}	T _{i,P}	H	T _{i,In} ^(a) (barrier)
LDA	+0.41	+0.25	0	<1.13	0	0.40	<1.09
LDA-3d	+0.37	+0.28	0	<1.09	0	0.38	<1.05
PBE	+0.32	+0.25	0	<1.25	0	0.34	<1.25
PBE-3d	n/c	n/c	n/c	n/c	n/c	n/c	n/c

(a) The value is an upper bound, as the symmetric T_d site is a local maximum, and diffusion barrier will skirt this along a lower-energy path through the interstice.

2.4.3. Athermal and recombination enhanced diffusion

Unlike the arsenic interstitial in GaAs, the phosphorus interstitial in InP will *not* diffuse athermally in p -type. The obvious Bourgoin-Corbett migration path driven by capture of carriers is:



is blocked because the $T_{i,In}$ is a local maximum, and has a higher energy than the H site.

The number of bistabilities in both native interstitials, with frequent changes in structures with charge state and multiple low energy competitive structures for each charge state, suggest a high likelihood for recombination-enhanced diffusion.

2.5. Neutral defect formation energies

This section summarized results of formation energies of neutral defects for InP. The earlier results showed only the overall ground state for each defect. In this section, all the metastable minima for neutral charge defects are listed, with their associated formation energies. For the purposes of designing an interatomic potential intended to model radiation-induced displacement cascades, accurately reproducing the energies of the primary defects accurately will be needed to faithfully reproduce the damage in the end-of-range.

The following table lists formation energies of the difference structures for neutral (uncharged) simple intrinsic defects, with a brief description of the atomic configuration. Figures representing these configuration can be found in PAS09. A more detailed listing of the core atoms in the defect structures is described in the Appendix. The computed formation energies are listed for each simulation context, should a specific “chemistry” be desired to follow, along with a “best” value, which simply reflects expert judgment about the strengths and weaknesses of the simulation contexts to hazard a weighted guess for the best value to incorporate in a training set to best describe nature.

Table 18. Formation energies of neutral defects for InP (in eV).

Defect	Description	Simulation context			
		LDA	LDA-3d	PBE	“Best”
v'_{In}	T_d	3.97	3.89	3.85	3.9
v^*_{In}	Site-shift: pair-In $v_P P_{\text{In}}$	3.00	3.06	2.81	2.9
v'_P	Resonant- D_{2d}	2.68	2.73	2.72	2.7
v^*_P	Site-shift: $v_P P_{\text{In}}$	Unstable			
$\nu\nu = \nu_P \nu_{\text{In}}$	C_{1h} : outward-In	4.33	4.33	3.80	3.8
	C_{3v} : inward-In	4.75	4.74	4.59	4.6
	C_{1h} : paired-In	4.74	4.74	4.56	4.6
$aP = P_{\text{In}}$	T_d	1.95	1.95	1.66	1.9
	$EL2$ -distorted C_{3v}	2.13	2.13	1.91	2.1
	C_{3v} TS between T_d — $EL2$	2.51	2.51	2.33	2.5
$a\text{In} = \text{In}_P$	Resonant- D_{2d}	2.81	3.07	3.13	3.1
	T_d	2.92	3.19	3.25	3.2
$aa = \text{In}_P P_{\text{In}}$	C_{3v}	2.54	2.80	2.71	2.7
$i\text{In} = \text{In}_i$	C_{2v} split-110 $_{\text{In}}$	4.11	4.19	4.21	4.2
	C_{2v} split-001 $_P$	4.51	4.67	4.68	4.7
	$T_d T_{i,P}$ (estimated) ^(a)	3.72	3.77	3.82	3.8
	$T_d T_{i,\text{In}}$ (estimated) ^(a)	3.68	3.81	3.85	3.8
$iP = P_i$	C_{2v} split-110 $_P$	3.12	3.11	2.95	3.1
	$C_{1h} T_{i,\text{In}}$ -side bent bridge	3.33	3.33	3.12	3.3
	D_{2d} split-001 $_P$	3.69	3.70	3.39	3.7
	C_{2v} split-001 $_{\text{In}}$	3.79	3.81	3.62	3.6
	$T_d T_{i,P}$	4.53	4.58	4.35	4.5
	$T_d T_{i,\text{In}}$	4.83	4.78	4.71	4.7

- (a) The DFT does not show a stable neutral defect in either T_i site. The value given is the formation energy of the interstitial at the CBE, equivalent to the energy of the neutral defect if the In_i were a shallow donor with the (0/+1) transition exactly at the CBE (arbitrarily set to be 1.42 eV above the VBE, i.e., the experimental gap over the nominal, uncalibrated position used for the VBE). These values should be used with some caution.

3. CONCLUSIONS

The parameters needed to describe the defect properties of simple intrinsic defects in InP are summarized into Tables. Indications from these calculations of where additional calculations and experiments could be targeted to further refine the defect physics model are listed, particularly for the identification and characterization of diffusive species.

4. REFERENCES

1. P.A. Schultz, Phys. Rev. Lett. **96**, 246401 (2006).
2. P.A. Schultz and O.A. von Lilienfeld, Modelling Simul. Mater. Sci. Eng. **17**, 084007 (2009).
3. SEQQUEST code, unpublished, <http://dft.sandia.gov/quest/>
4. J.P. Perdew and A. Zunger, Phys. Rev. **23**, 5048 (1981).
5. J.P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).
6. A.E. Mattsson, P.A. Schultz, M.P. Desjarlais, T.R. Mattsson, and K. Leung, Modelling Simul. Mater. Sci. Eng. **13**, R1 (2005).
7. P.A. Schultz, Phys. Rev. B **60**, 1551 (1999).
8. O.A. von Lilienfeld and P.A. Schultz, Phys. Rev. B **77**, 115202 (2008).
9. D.R. Hamann, Phys. Rev. B **40**, 2980 (1989).
10. S.G. Louie, S. Froyen, and M.L. Cohen, Phys. Rev. B **26**, 1738 (1982).
11. P. Deus, H.A. Schneider, H. Voland, and K. Stiehler, phys. stat. sol. (a) **108**, 443 (1987).
12. F.S. Hickernell and W.R. Gayton, J. Appl. Phys. **37**, 462 (1966)..
13. W.J. Turner, W.E. Reese, and G.D. Petit, Phys. Rev. **136**, A1467 (1964).
14. V.P Vasil'ev and J.-C. Gachon, Inorg. Mat. **42**, 1171 (2006).
15. W. Jost, J. Chem. Phys. **1**, 466 (1933).
16. R.E. Neidert, S.C. Binari, and T. Weng, Electron. Lett. **18**, 987 (1982).
17. G.D. Watkins, in *Radiation Damage in Semiconductors*, ed. P. Baruch, p97 (Paris:Dunod, 1965).
18. J.C. Bourgoin and J.W. Corbett, Phys. Lett. A **38**, 135 (1972).

This page intentionally left blank

APPENDIX A: NEUTRAL DEFECT ATOMIC CONFIGURATIONS

The configuration of the core atoms in the neutral defects is listed in this section, to more precisely define the atomic configurations associated with the ground state descriptions in Table 18. The defect site(s) and the first nearest neighbor shell are included in the listing, for relaxed defect structures within the LDA simulation context. The coordinates are given as Cartesian coordinates, in units of lattice constants. The name associated with the data file corresponding to the atomic configuration relaxed calculation is also included.

v'_{In}		$vIn_0_Td_tdC$			v^*_{In}		$vaP_0_Cspair_tdA$		
Symmetric T_d		Origin: In-site			Site-shift pair-In v_pP_{In}		Origin: P-site		
vac_In	vac	0.0000	0.0000	0.0000	vac_P	vac	0.0000	0.0000	0.0000
AT0002	P	0.2124	0.2124	0.2124	anti_In	P	0.2468	0.2468	0.2521
AT0003	P	0.2124	-0.2124	-0.2124	AT0003	In	0.1749	-0.1953	-0.2349
AT0004	P	-0.2124	0.2124	-0.2124	AT0004	In	0.1953	0.1749	-0.2349
AT0005	P	-0.2124	-0.2124	0.2124	AT0005	In	-0.2198	-0.2198	0.2060
v'_P		$vP_0_D2d_tdA$			vv		$vv_0_C3vout_tdA$		
Resonant- D_{2d}		Origin: P-site			C_{3v} : outward-In		Origin: P-site		
vac_P	vac	0.0000	0.0000	0.0000	vac_P	vac	0.0000	0.0000	0.0000
AT0002	In	0.2028	0.2028	0.2476	vac_In	vac	0.2500	0.2500	0.2500
AT0003	In	0.2028	-0.2028	-0.2476	AT0003	In	0.3085	-0.2966	-0.2966
AT0004	In	-0.2028	0.2028	-0.2476	AT0004	In	-0.2966	0.3085	-0.2966
AT0005	In	-0.2028	-0.2028	0.2476	AT0005	In	-0.2966	-0.2966	0.3085
					AT0006	P	0.4602	0.4602	0.0411
					AT0007	P	0.4602	0.0411	0.4602
					AT0008	P	0.0411	0.4602	0.4602
vv		$vv_0_C3v_tdA$			vv		$vv_0_Cspair_tdA$		
C_{3v} : inward-In		Origin: P-site			C_{1h} : paired-In		Origin: P-site		
vac_P	vac	0.0000	0.0000	0.0000	vac_P	vac	0.0000	0.0000	0.0000
vac_In	vac	0.2500	0.2500	0.2500	vac_In	vac	0.2500	0.2500	0.2500
AT0003	In	0.2033	-0.2248	-0.2248	AT0003	In	0.1861	-0.1929	-0.2312
AT0004	In	-0.2248	0.2033	-0.2248	AT0004	In	-0.1929	0.1861	-0.2312
AT0005	In	-0.2248	-0.2248	0.2033	AT0005	In	-0.2715	-0.2715	0.2657
AT0006	P	0.4662	0.4662	0.0475	AT0006	P	0.4627	0.4627	0.0433
AT0007	P	0.4662	0.0475	0.4662	AT0007	P	0.4592	0.0502	0.4723
AT0008	P	0.0475	0.4662	0.4662	AT0008	P	0.0502	0.4592	0.4723

P _{In}		aP_0_Td_tdC			P _{In}		aP_0_C3vfar_tdC		
T _d phosphorus antisite			Origin: In-site		C _{3v} -distorted (EL2*)			Origin: In-site	
anti_In	P	0.0000	0.0000	0.0000	anti_In	P	-0.1301	-0.1301	-0.1301
AT0002	P	0.2391	0.2391	0.2391	AT0002	P	0.2155	0.2155	0.2155
AT0003	P	0.2391	-0.2391	-0.2391	AT0003	P	0.2256	-0.2359	-0.2359
AT0004	P	-0.2391	0.2391	-0.2391	AT0004	P	-0.2359	0.2256	-0.2359
AT0005	P	-0.2391	-0.2391	0.2391	AT0005	P	-0.2359	-0.2359	0.2256
P _{In}		aP_0_C3vTS_tdC			In _P		aIn_0_D2dres_tdA		
C _{3v} -transition state			Origin: In-site		Resonant- D _{2d}			Origin: P-site	
anti_In	P	-0.0712	-0.0712	-0.0712	anti_P	In	0.0000	0.0000	0.0000
AT0002	P	0.1993	0.1993	0.1993	AT0002	In	0.2753	0.2753	0.2346
AT0003	P	0.2527	-0.2359	-0.2359	AT0003	In	0.2753	-0.2753	-0.2346
AT0004	P	-0.2359	0.2527	-0.2359	AT0004	In	-0.2753	0.2753	-0.2346
AT0005	P	-0.2359	-0.2359	0.2527	AT0005	In	-0.2753	-0.2753	0.2346
In _P		aIn_0_Td_tdA			aa		aa_0_C3v_tdA		
Symmetric T _d			Origin: P-site		Symmetric C _{3v}			Origin: P-site	
anti_P	In	0.0000	0.0000	0.0000	anti_P	In	0.0103	0.0103	0.0103
AT0002	In	0.2619	0.2619	0.2619	anti_In	P	0.2599	0.2599	0.2599
AT0003	In	0.2619	-0.2619	-0.2619	AT0003	In	0.2616	-0.2492	-0.2492
AT0004	In	-0.2619	0.2619	-0.2619	AT0004	In	-0.2492	0.2616	-0.2492
AT0005	In	-0.2619	-0.2619	0.2619	AT0005	In	-0.2492	-0.2492	0.2616
					AT0006	P	0.4827	0.4827	0.0327
					AT0007	P	0.4827	0.0327	0.4827
In _i		iIn_0_110iC2v_tdC			In _i		iIn_0_001pC2v_tdA		
C _{2v} -split-110 _{In}			Origin: In-site		C _{2v} -split-001 _P			Origin: P-site	
split1	In	0.1769	0.1769	-0.1390	intl_In	In	0.0000	0.0000	0.0538
split2	In	-0.1769	-0.1769	-0.1390	AT0001	P	0.0000	0.0000	-0.3601
AT0002	P	0.2689	0.2689	0.2742	AT0002	In	0.2765	0.2765	0.2661
AT0003	P	0.2648	-0.2648	-0.2709	AT0003	In	0.3018	-0.3018	-0.2874
AT0004	P	-0.2648	0.2648	-0.2709	AT0004	In	-0.3018	0.3018	-0.2874
AT000	P	-0.2689	-0.2689	0.2742	AT0005	In	-0.2765	-0.2765	0.2661

In _i		iIn_0_TipTd_tiA			In _i		iIn_0_TiiTd_tiC		
T _d symmetry T _{i,P} site		Origin: T _{i,P} site			T _d symmetry T _{i,In} site		Origin T _{i,In} site		
intl_In	In	0.0000	0.0000	0.0000	intl_In	In	0.0000	0.0000	0.0000
AT0001	P	0.2640	0.2640	0.2640	AT0001	In	0.2785	0.2785	0.2785
AT0002	P	0.2640	-0.2640	-0.2640	AT0002	In	0.2785	-0.2785	-0.2785
AT0003	P	-0.2640	0.2640	-0.2640	AT0003	In	-0.2785	0.2785	-0.2785
AT0004	P	-0.2640	-0.2640	0.2640	AT0004	In	-0.2785	-0.2785	0.2785
P _i		P_0_110pC2v_tdA			P _i		iP_0_BiCs_tdA		
C _{2v} split-110 _p		Origin: P-site			C _{1h} T _{i,In} -side bent bridge		Origin: P-site		
split1	P	0.1311	0.1311	-0.0864	intl_P	P	0.0357	0.0357	0.2725
split2	P	-0.1311	-0.1311	-0.0864	AT0001	P	-0.0790	-0.0790	-0.0518
AT0002	In	0.2737	0.2737	0.2833	AT0002	In	0.3255	0.3255	0.2785
AT0003	In	0.2686	-0.2686	-0.2760	AT0003	In	0.2527	-0.2625	-0.2616
AT0004	In	-0.2686	0.2686	-0.2760	AT0004	In	-0.2625	0.2527	-0.2616
AT0005	In	-0.2737	-0.2737	0.2833	AT0005	In	-0.3047	-0.3047	0.2535
P _i		iP_0_001pD2d_tdA			P _i		iP_0_001iC2v_tdC		
D _{2d} split-001 _p		Origin: P-site			C _{2v} split-001 _{in}		Origin: In-site		
split1	P	0.0000	0.0000	0.1757	intl_P	P	0.0000	0.0000	0.3165
split2	P	0.0000	0.0000	-0.1757	AT0001	In	0.0000	0.0000	-0.0895
AT0002	In	0.2827	0.2827	0.3020	AT0002	P	0.2871	0.2871	0.2784
AT0003	In	0.2827	-0.2827	-0.3020	AT0003	P	0.2640	-0.2640	-0.2855
AT0004	In	-0.2827	0.2827	-0.3020	AT0004	P	-0.2640	0.2640	-0.2855
AT0005	In	-0.2827	-0.2827	0.3020	AT0005	P	-0.2871	-0.2871	0.2784
P _i		iP_0_TipTd_tiA			P _i		iP_0_TiiTd_tiC		
T _d symmetry T _{i,P} site		Origin: T _{i,P} site			T _d symmetry T _{i,In} site		Origin T _{i,In} site		
intl_P	P	0.0000	0.0000	0.0000	intl_P	P	0.0000	0.0000	0.0000
AT0001	P	0.2375	0.2375	0.2375	AT0001	In	0.2601	0.2601	0.2601
AT0002	P	0.2375	-0.2375	-0.2375	AT0002	In	0.2601	-0.2601	-0.2601
AT0003	P	-0.2375	0.2375	-0.2375	AT0003	In	-0.2601	0.2601	-0.2601
AT0004	P	-0.2375	-0.2375	0.2375	AT0004	In	-0.2601	-0.2601	0.2601
END ATOMIC CONFIGURATIONS									

DISTRIBUTION

(to be distributed electronically)

1	MS0899	Technical Library	9536 (electronic copy)
1	MS1179	L. J. Lorence	1341 (ljloren@sandia.gov)
1	MS1056	W. R. Wampler	1111 (wrwampl@sandia.gov)
1	MS1323	E. R. Keiter	1445 (erkeite@sandia.gov)
1	MS1315	J. S. Nelson	1131 (jsnelso@sandia.gov)
1	MS1189	T. R. Mattsson	1641 (trmatts@sandia.gov)
1	MS0457	R. A. Paulsen	2211 (rapauls@sandia.gov)
1	MS1415	A. F. Wright	1131 (afwrigh@sandia.gov)
1	MS1411	S. M. Foiles	1814 (foiles@sandia.gov)
1	MS1322	A. P. Thompson	1425 (athomps@sandia.gov)

