

CCC-4 Proposal**Principal Investigator:**

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Lab/Department/Division/Group: Sandia National Laboratories/1100/1131

Please provide a one-line unclassified title for this proposal: *Density-functional-theory calculations of point-defect diffusion pathways and activation energies*

Milestones supported (if any): ASC Level 3 milestone for the Qualification Alternative to the Sandia Pulsed Reactor (QASPR) Project

Goal/Objective: Use density-functional theory to identify the diffusion pathways of indium and phosphorous interstitials in indium phosphide. These results will be used to model gain degradation and recovery in group III-V based semiconductor transistors for the QASPR Project.

Readiness Justification - Scaling: Scaling: A plot of $\log_2(\text{wall-time})$ vs. $\log_2(\# \text{ of cores})$ from results obtained on Cielo yielded a slope of -0.82 (where ideal scaling would be -1). This scaling is valid for run sizes up to $100 * \text{ns} * \text{nc}$ nodes (all cores/node utilized), where ns is the number of sampling points (4 – 14) and nc is the number of atomic configurations (2 – 7).

Experience:**C1 Requirements (jobs that use 6375 or more nodes)**

Number of jobs in this category that will be run: 4

Size (number of nodes needed): 8100

Average run time for jobs in this category: 24 hours

Code used: Socorro

C2 Requirements (jobs that use at least 2550 but less than 6374 nodes)

Number of jobs in this category that will be run: 10

Size (number of nodes needed): 2700

Average run time for jobs in this category: 24 hours

Code used: Socorro

C3 Requirements (jobs that use at least 850 but less than 2549 nodes)

Number of jobs in this category that will be run: 2000, 1200, 1000

Size (number of nodes needed): 12, 18, 20

Average run time for jobs in this category: 24 hours

Code used: Socorro

Based on your C-level requirements, please provide the total number of Cielo days' allocation required to fulfill your proposal requests. Base your aggregation calculations on: 8518 compute nodes for 24 hours = 1 Cielo day. Total Cielo days required for this proposal is: 12

Data Management:

Based on your C-level requirements, please provide estimates for the following:

How much data do you expect to store in the /scratch file system? (< 1 TB)

How much data do you expect to store in the LANL HPSS archive? (0 TB)

How much data do you expect to transfer across the WAN? (0 TB)

For data to be transferred across the WAN: will it be destined for a file system, HPSS, or both?

Will your application require the use of the read-only "UDSL" file system? No
If so, please estimate the size of the data storage required (GB).

Application Codes and Application Development Teams

Please list the application codes that you will be running on Cielo during the campaign. Socorro

Please list the primary contact for each application development/support team for the applications you plan to run. Alan F. Wright

Visualization

What visualization software/tools will you require on Cielo? None

List of users authorized to use this CCC bank. Please specify each user's name, login name, e-mail address, and work phone:

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