EPSRC UK National Service for Computational Chemistry Software at Imperial College London

Funding period: 1st February 2011 – 31st January 2017
EPSRC Reference: EP/J003921/1

Key Performance Indicators (KPI) for the period of 1st February 2016 to 31st January 2017

	Feb-Apr 2016	**May-Jul 2016**	**Aug-Oct 2016**	**Nov 2016-Jan 2017**
A) No. of Separate Uni. Res. Group	73	75	65	55
B) Percentage Uptime of Total Available Time	99.72%	99.66%	99.60%	99.64%
C) Percentage of Training Requests Responded to within Stated Window	100%	100%	100%	100%
D) Percentage of Training Requests Delivered within Stated Window	100%	100%	100%	100%
E) Percentage of Computer Access Requests Responded to within Stated Window	100%	100%	100%	100%
F) Percentage of Computer Access Requests Accepted	100%	100%	100%	100%
G) Average / Peak Loading	Slater 57.07% / 108.55%	Slater 56.91% / 117.19%	Slater 44.58% / 87.76%	Slater 59.91% / 94.07%
H) Number of Customer Complaints / Approvals*	0/0	0/0	0/0	0/0
I) Number of Publications**	30	16	6	0

*No complaints/approvals received from users. **Publications reported during the period (See 2_Publications_Reported_Year6.pdf for a full list). ^^More processes eligible to run than available CPUs. If there are more threads than CPUs some threads will have to wait for a slice of a CPU to be allotted before that can do anything and the load average will be greater than the number of CPUs.

The KPIs are:

A) The Number of Individual Researchers and University Research Groups ["Users"] that have been in contact with Imperial College regarding EPSRC UK NSCCS (e.g. for advice, guidance etc) and/or

have made use of the EPSRC UK NSCCS Service in that Period. This should be expressed as a Total Number for that period (If it is possible to split the total number into EPSRC UK NSCCS Users and EPSRC UK NSCCS Enquiries then this would be advantageous). The number reported is that of "Users" which have made use of the EPSRC UK NSCCS Service in that Period.

(The number reported is the total number of separate university research groups using the NSCCS during the period. This number does not include people who attended NSCCS Workshops that were opened to any UK academic staff, students and non-UK and non-academics. See 3_Summary_of_Training_Events_Year6.pdf for full details of all training events.)

B) The Uptime (or Downtime) of the EPSRC UK NSCCS Equipment within the period.

This will be expressed as a percentage of the Total Available Time within that Period.

C) Percentage of Training Requests Responded to within Stated Window

D) Percentage of Training Requests Delivered within Stated Window

E) Percentage of Computer Access Requests Responded to within Stated Window

F) Percentage of Computer Access Requests Accepted

G) Average / Peak Loading (See Figures 1 & 2 for details)

H) Number of Customer Complaints / Approvals

I) Number of Publications (including examples of Key Publications with acknowledgement of EPSRC UK NSCCS Service) (See 2_Publications_Reported_Year6.pdf)

J) Annual Data - Identification & Load of Software usage (See Figure 3 for details)

K) Annual Data - Identification of Spectrum of Users Types & Departmental Affiliation (See Figures 4 to 6 for details)

G) Average / Peak Loading

The ganglia load graph shown in Figure 1 gives the load (CPUs in use) of the machine for the period of 1st February 2016 to 31st January 2017.

Figure 2 show the CPU time used via the queuing systems for the period of 1st February 2016 to 31st January 2017.

Slater

The Altix UV2000 has 512 CPUs with 480 dedicated to batch work. This gives 80,640 hours a week. Working on an overall average for the year of 98% of time being scheduled availability, i.e. approx. 8 days a year outage for scheduled developments, etc., this gives 78,868 as the weekly available hours.
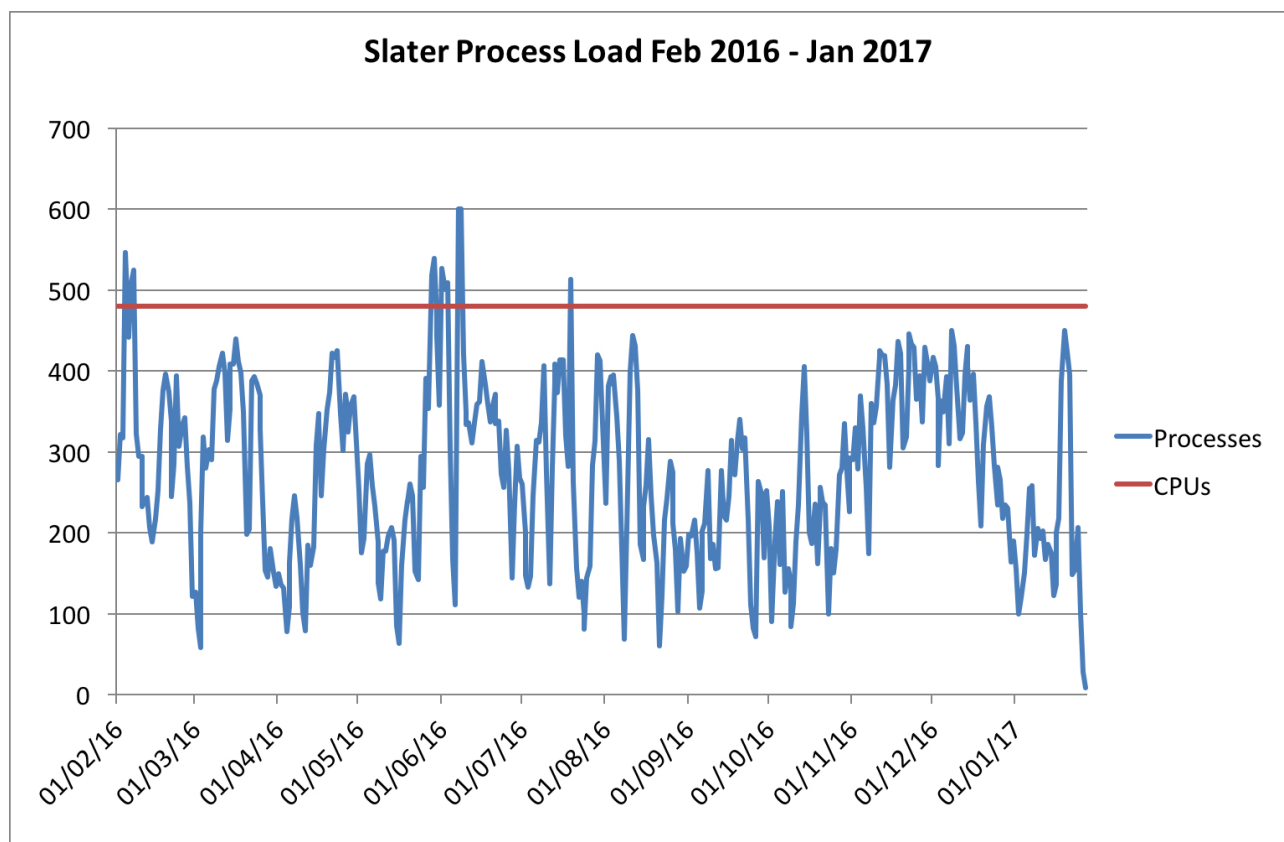

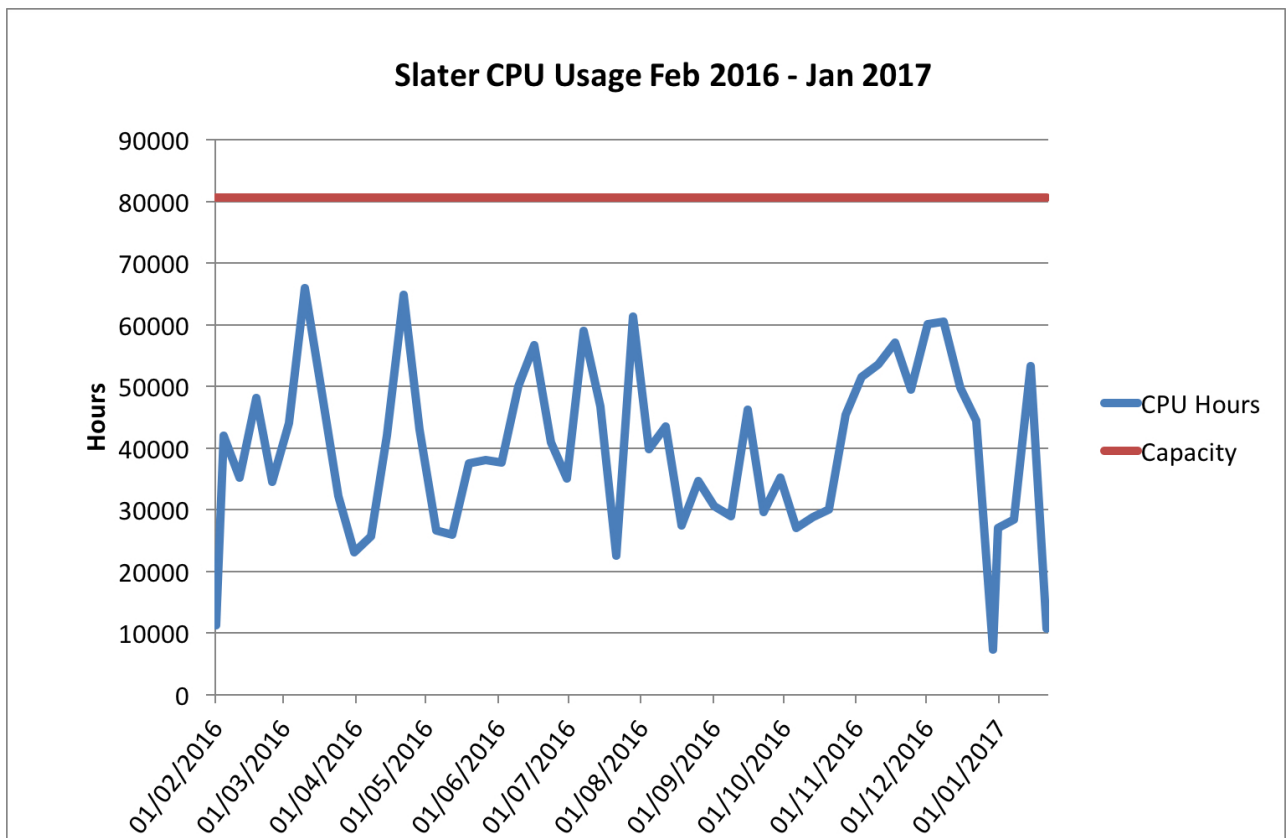Figure 1. Ganglia load of NSCCS machine (Slater).

Figure 2. CPU usage of NSCCS machine (Slater).

J) Annual Data - Identification & Load of Software usage

The most used software package in terms of computing processing unit (CPU) is Gaussian at 66.49% as shown in Figure 3. The list of software packages' usage as a percentage is shown in Table 1.

*Please note that this is only for illustrative purpose since the logusage script used to gather the data cannot account for all parallel CPU usage. However, the actual CPU usage would have been accounted for by the system.
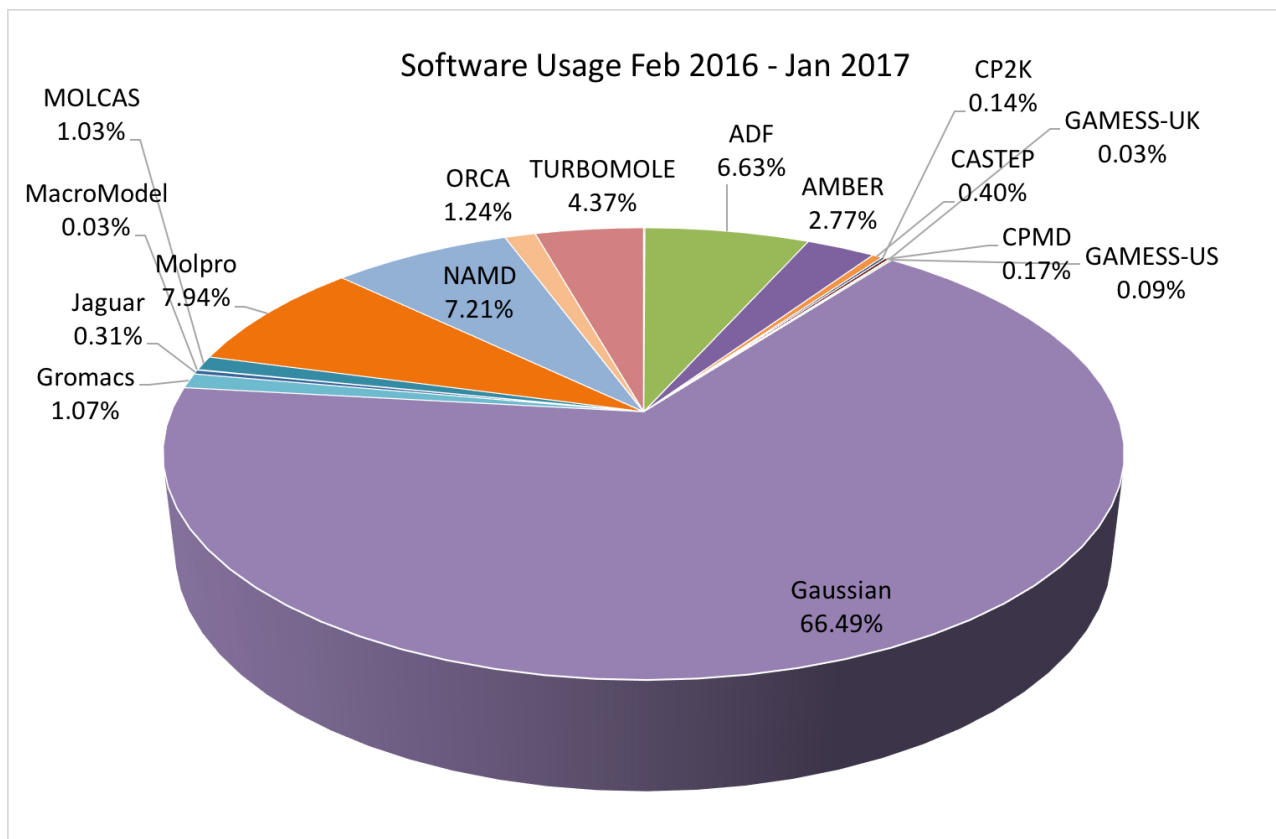

Figure 3. Software Usage for the period of 1st Feb 2016 to 31st January 2017.

Software	Software Usage (%)
ACES	0.05
ADF	6.63
AMBER	2.77
CASTEP	0.40
CP2K	0.14
CPMD	0.17
CRYSTAL	0.01
GAMESS-UK	0.03
GAMESS-US	0.09
Gaussian	66.49
Gromacs	1.07
Jaguar	0.31
LAMMPS	0.01
MacroModel	0.03
MOLCAS	1.03
Molpro	7.94
NAMD	7.21
ORCA	1.24
TURBOMOLE	4.37

Table 1. List of software packages' usage for the period of 1st Feb 2016 to 31st January 2017.

K) Annual Data - Identification of Spectrum of Users Types & Departmental Affiliation

The NSCCS received 38 applications during the period of 1st February 2016 to 31st January 2017 with 9 pump-priming applications and 28 full applications with one rejected application; from 31 separate research groups from 18 institutions. Due to uncertainties to the future of service this had a significant impact resulting in the reduction of applications received. The service stopped accepting new applications on the 9th November 2016 in preparation for the closing of service on the 31st January 2017.

Figure 4 gives a breakdown of the number of research groups per institution from the 37 approved applications. The pie charts in Figures 5 & 6 illustrate the percentages of the different departments and different research categories of the research groups of these applications.
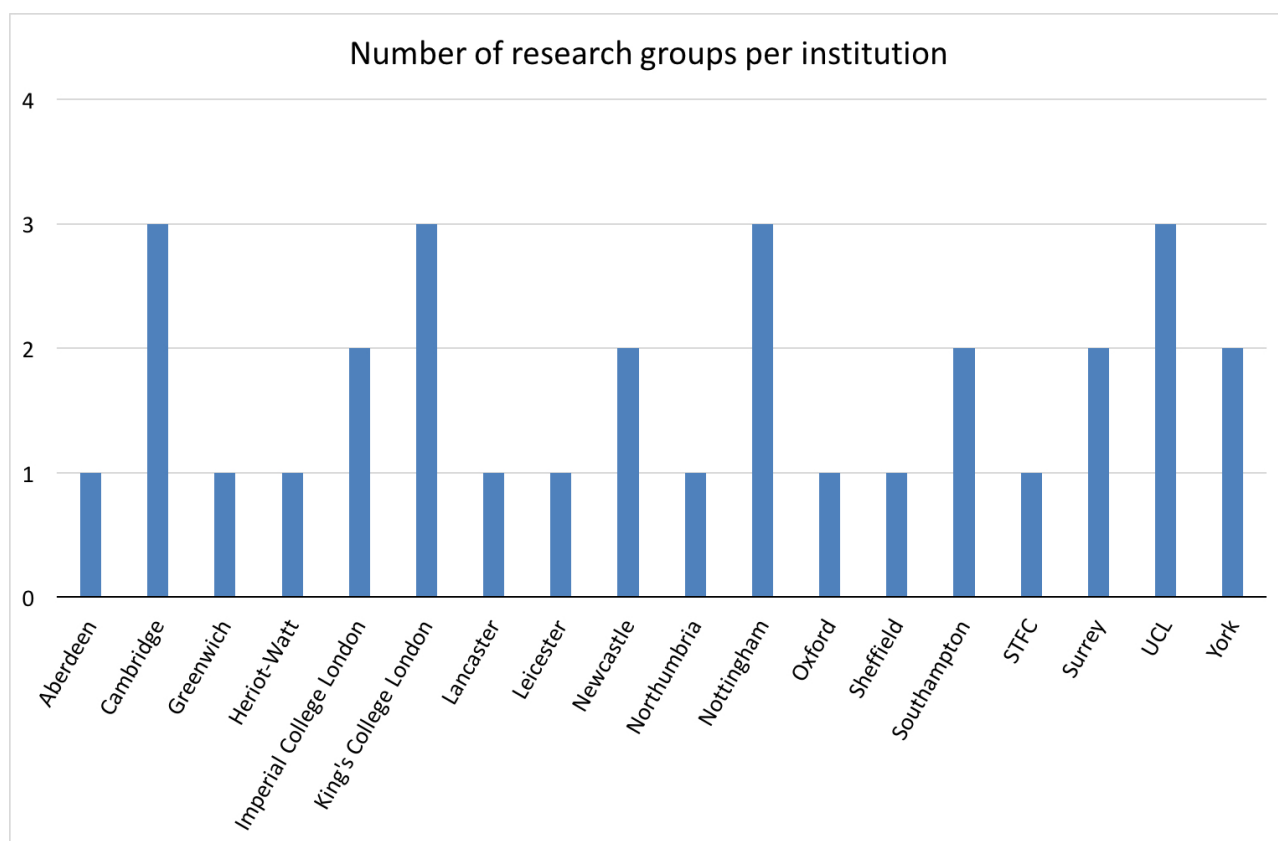

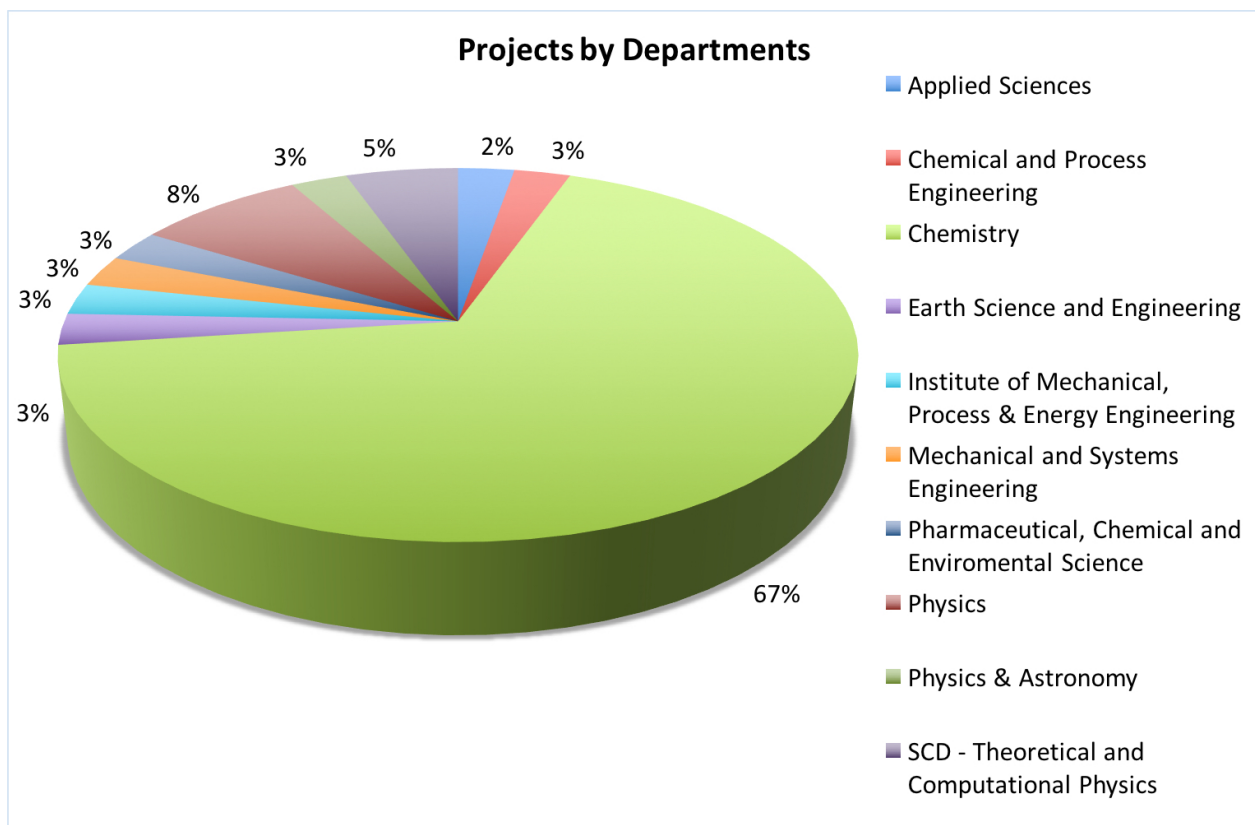Figure 4. Number of research groups per institution.
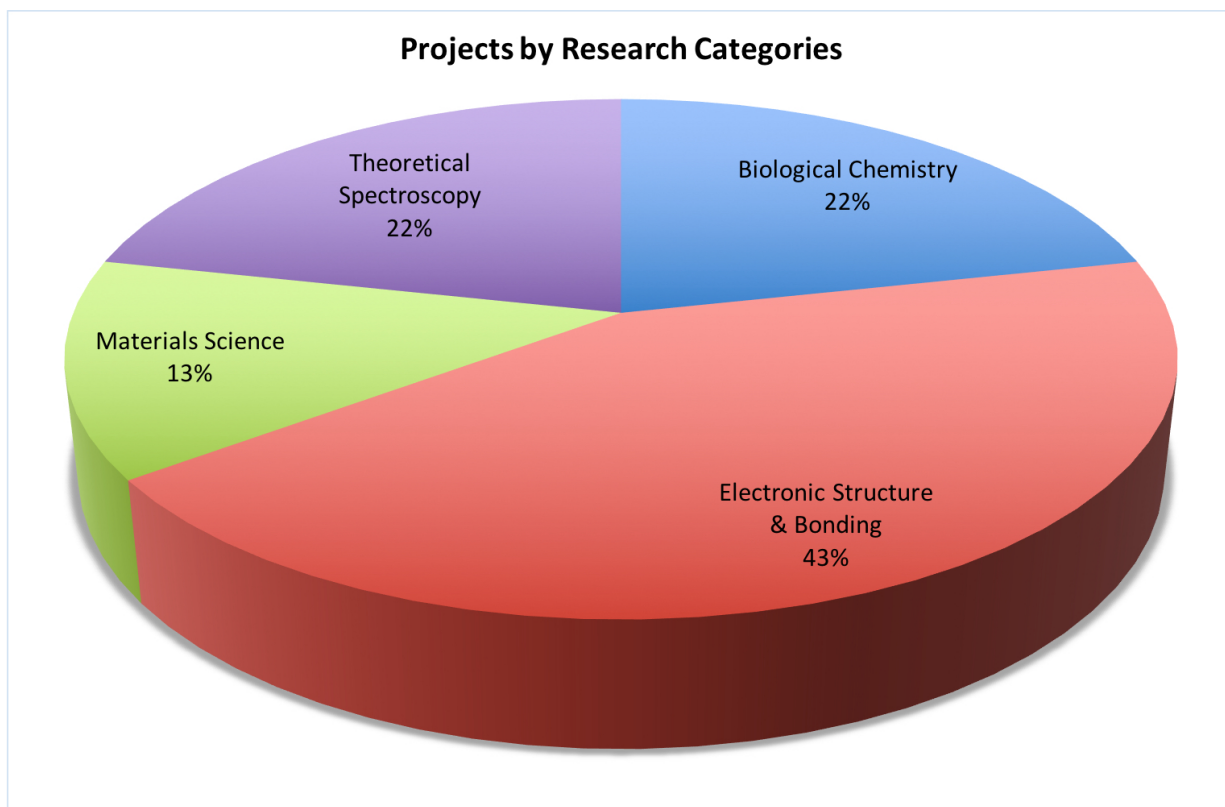
Figure 5. Users' department listed as a percentage.

Figure 6. Research categories listed as a percentage.