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

Key Performance Indices (KPI) for the period of 1st February 2013 to 31st January 2014

	Feb-Apr	May-Jul	Aug-Oct	Nov-Jan
A) No. of Separate Uni. Res. Group	59	74	81	83
B) Percentage Uptime of Total Available Time	97.2% (Columbus)	99.3% (Columbus)	99.3% (Columbus)	100% (Columbus)
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	300(59%)/524(102%) (Columbus) ^^	291(57%)/442(86%) (Columbus)	200(39%)/435(85%) (Columbus)	309(60%)/454(89%) (Columbus)
H) Number of Customer Complaints / Approvals*	0/0	0/0	0/0	0/0
I) Number of Publications**	28	22	14	10

*No complaints/approvals received from users. An annual user survey has been sent to users (See 4_NSCCS Annual User Satisfaction Survey 2014.pdf for details.)   **Publications reported during the period (See 2_Publications_Reported_Year3.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.

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 1-4 for details)

H) Number of Customer Complaints / Approvals (See 4_NSCCS Annual User Satisfaction Survey 2014.pdf)

I) Number of Publications (including examples of Key Publications with acknowledgement of EPSRC UK NSCCS Service) (See 2_Publications_Reported_Year3.pdf)

J) Annual Data - Identification & Load of Software usage (See Figure 5 for details)

K) Annual Data - Identification of Spectrum of Users Types & Departmental Affiliation (See Figures 6-8 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 2013 to 31st January 2014.

Figure 2 shows the CPU time used via the queuing systems for the period of 1st February 2013 to 31st January 2014.

Columbus

The Altix UV1000 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.
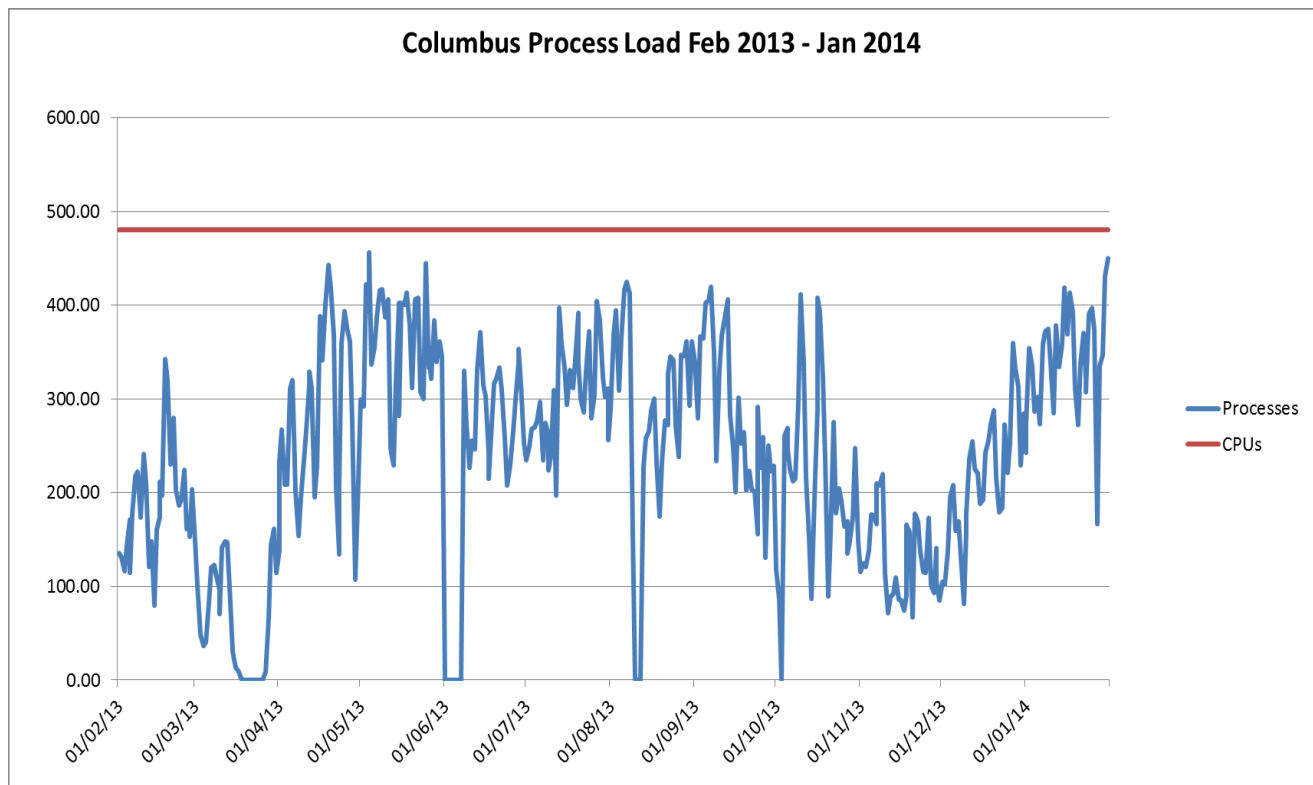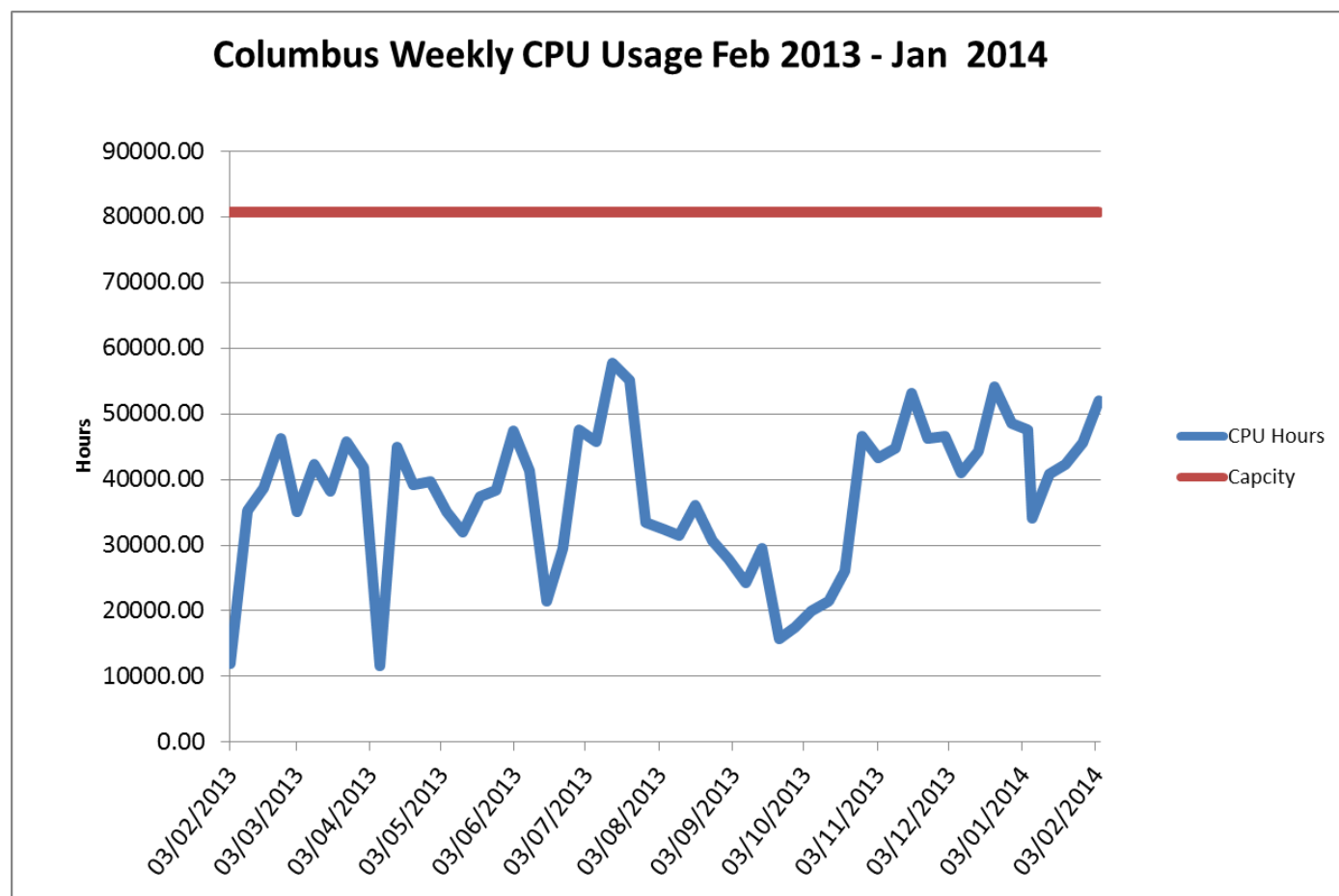
Figure 1. Ganglia load of NSCCS machine (Columbus).

Figure 1 caption: Columbus Process Load Feb 2013 - Jan 2014

Figure 2. LSF batch load of NSCCS machine (Columbus).

Columbus Weekly CPU Usage Feb 2013 - Jan 2014

J) Annual Data - Identification & Load of Software usage

The most used software package in terms of computing processing unit (CPU) is Gaussian at 73% as shown in Figure 3.

*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.
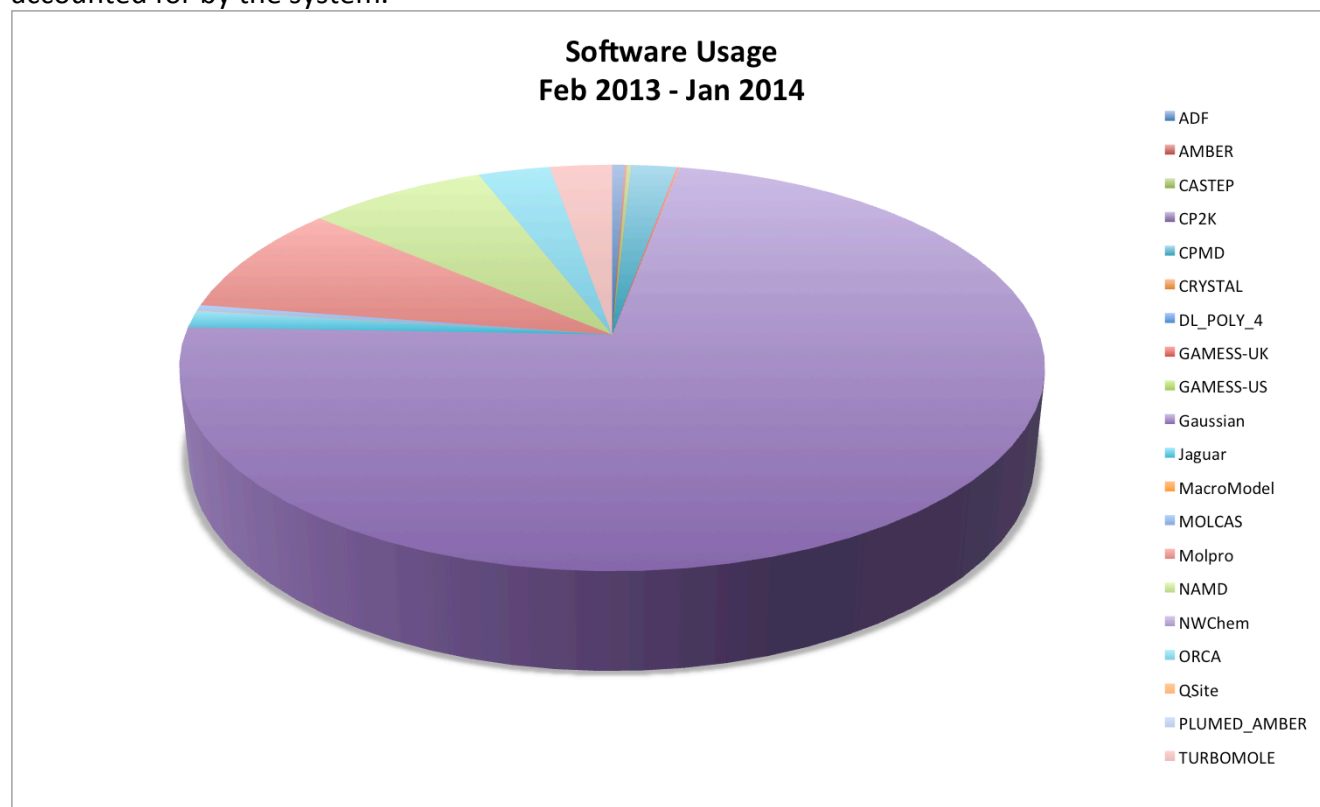

Figure 3. Software usage for the period of 1st Feb 2013 to 31st January 2014.

Software	Software Usage (%)	Software	Software Usage (%)
ADF	0.5360	Jaguar	1.3456
AMBER	0.1092	MacroModel	0.0546
CASTEP	0.1920	MOLCAS	0.4478
CP2K	0.0143	Molpro	8.8394
CPMD	1.9653	NAMD	7.8439
CRYSTAL	0.0023	NWChem	0.0000
DL_POLY_4	0.0019	ORCA	3.1457
GAMESS-UK	0.1141	QSite	0.0000
GAMESS-US	0.0124	PLUMED_AMBER	0.0001
Gaussian	72.6525	TURBOMOLE	2.7229

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

The NSCCS received 79 applications during the second year – 24 pump-priming applications and 55 full applications, two were rejected, from 64 separate research groups from 37 institutions.

Figure 4 gives a break down of research groups per institution. The pie charts in Figures 5 & 6 illustrate the percentages of the different departments and different research categories of the research groups.
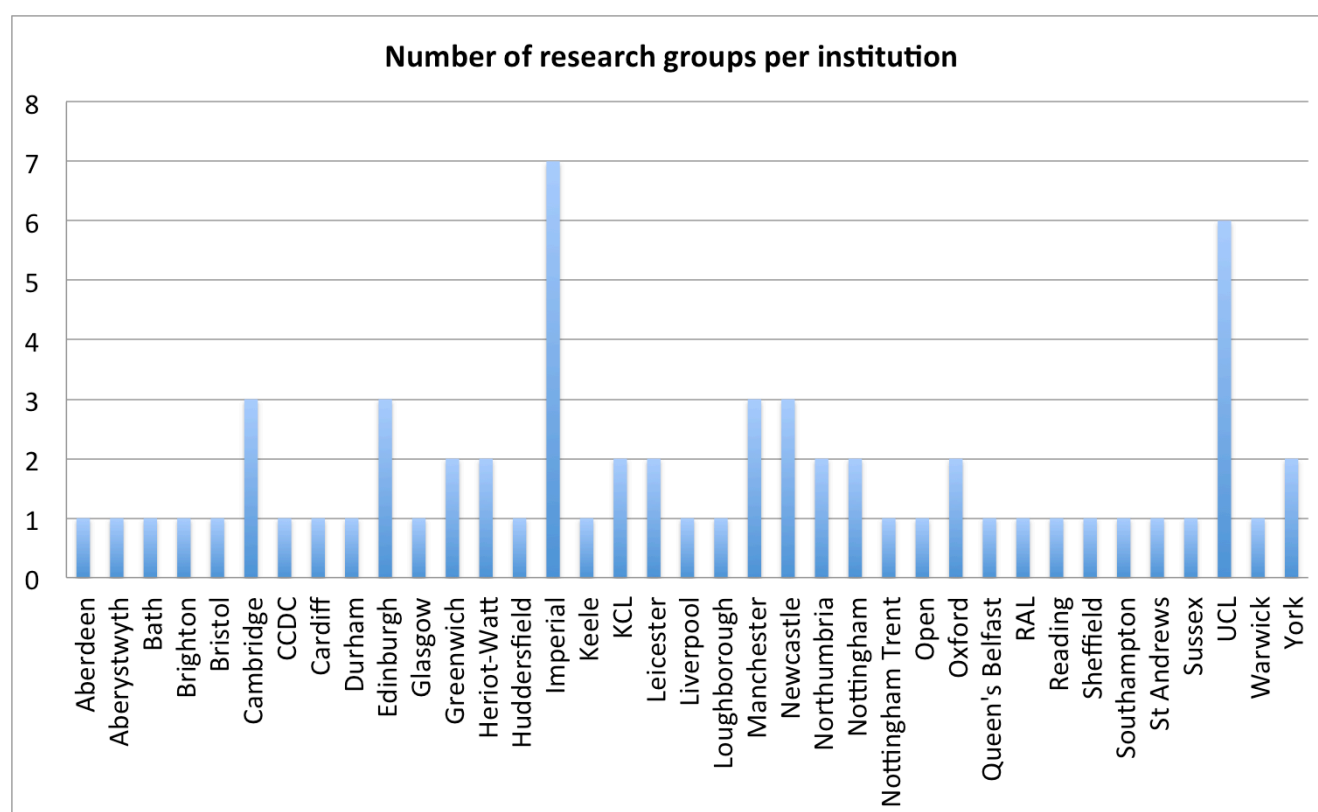

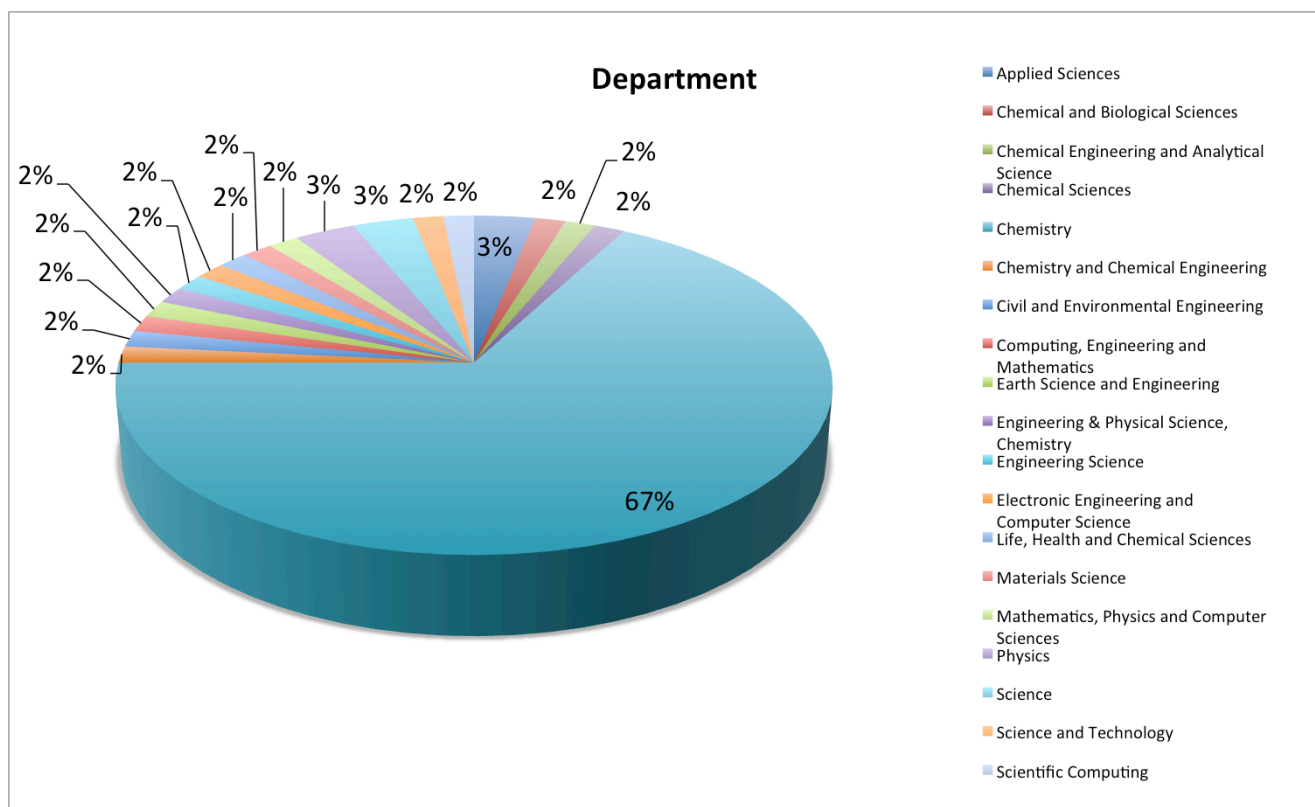**Figure 4. Number of research groups per institution.**
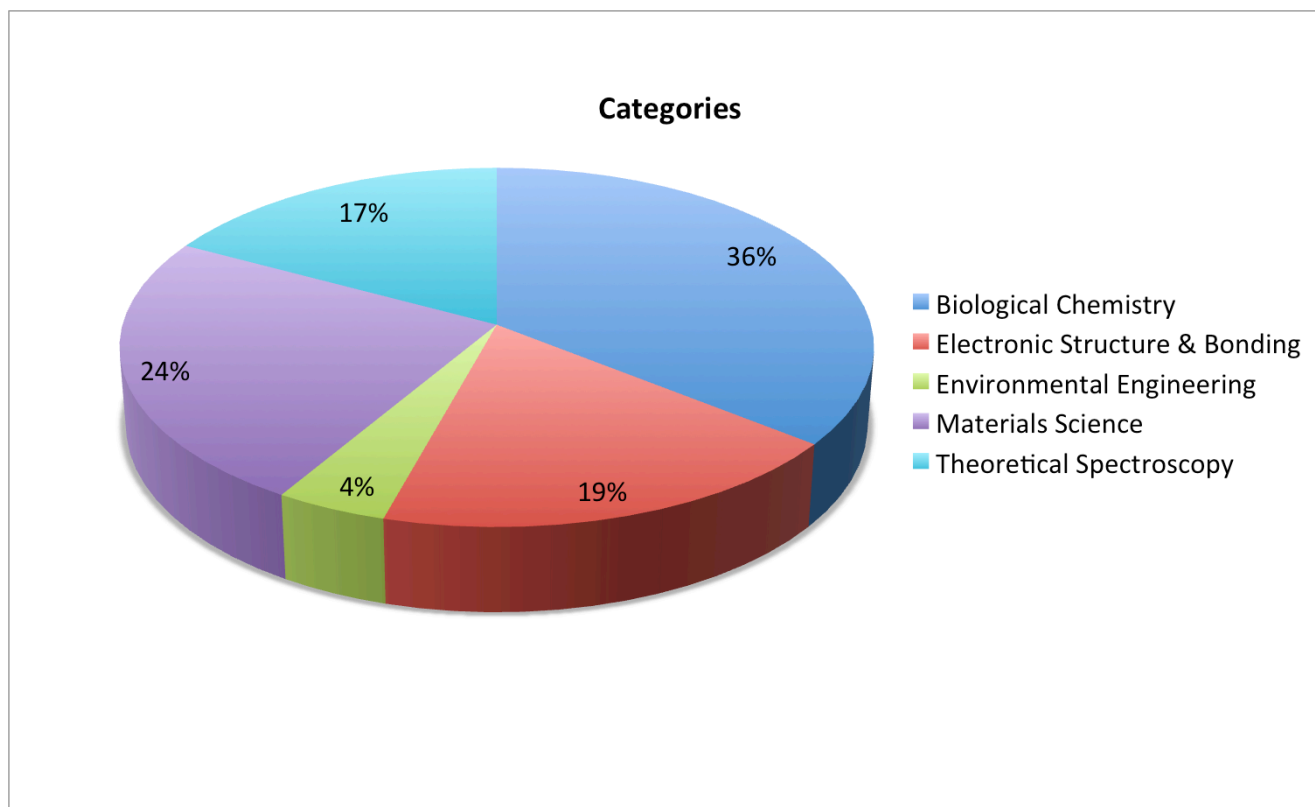
Figure 5. Users' Department listed as a percentage.

Figure 6. Research categories listed as a percentage.