Abstract Information

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Principal Investigator(PI):* Teri W. Odom
PI Department:* Chemistry
Abstract Title:* Superlattice Plasmons in Hierarchical Nanoparticle Arrays
Computational Resources:* Quest

Abstract:

Periodic metal nanoparticle (NP) arrays support narrow lattice plasmon resonances that can be tuned by changing the localized surface plasmons of the individual NPs in the array, NP periodicity, and dielectric environment. Here we report superlattice plasmons that can be supported by hierarchical Au NP arrays, where finite arrays of NPs (patches) are organized into arrays with larger periodicities. We show that superlattice plasmons can be described by the coupling of single-patch lattice plasmons and Bragg modes defined by the patch periodicity. Moreover, we identified the specific Bragg modes that contributed to the superlattice resonances by simulating both far-field transmission and near-field properties with finite-difference time-domain (FDTD) simulations. Superlattice plasmon resonances are often significantly narrower than that of single-patch lattice plasmon resonances and exhibit stronger local peak fields. By varying the periodicity of the patches, we demonstrated that the number and spectral location of superlattice plasmon resonances can be tailored in hierarchical Au NP arrays. These narrow superlattice plasmon resonances open prospects in ultrasensitive sensing and energy transfer and plasmon amplification in plasmonic cavities.
Abstract Information

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Abstract Title: * Angular Momentum Transport in Protoplanetary Disks: Planet Formation on GPUs.
Computational Resources: * Quest

Abstract:

For the first time ever, we can directly see the imprints of young planets on their environments. Large sub-millimeter interferometric arrays such as ALMA have opened a new chapter on planet formation by providing us with unprecedented observations of gas and dust in protoplanetary disks. In particular, the observed brightness distribution in the disk can be compared against detailed (magneto-)hydrodynamical simulations of massive planets interacting with the gas and dust surrounding them. Alternatively, one-dimensional models approximate how angular momentum is transferred from resonant spiral waves into the mean flow of the disk, which ultimately create deep gaps around the planet. One-dimensional models have the benefits of being both computationally inexpensive and physically enlightening. We are investigating how different angular momentum transfer functions compare against hydrodynamical simulations run with the FARGO3D code. Our simulations are run on the Quest computing cluster at Northwestern, where we utilize Nvidia Tesla K40 GPUs. One-dimensional models predict that a steady-state solution exists where the mass flux throughout the disk is constant. This implies that the viscous stresses which internally redistribute angular momentum are balanced by the planetary torques which deposit (extract) angular momentum exterior (interior) to the planet. For high mass planets and low disk viscosities, gas must pile-up exterior to the planet in order to overcome the repulsive tidal barrier. However, non-local deposition of this planetary angular momentum has the potential to reduce these observable pile-ups. Moreover, our hydrodynamical simulations are shedding light on the importance of these non-local processes, allowing us to accurately predict the properties of unseen planets from simplified models. In the near future, we will be running 3D simulations to better constrain the angular momentum transport processes as well as investigating the orbital migration of planets in low-mass disks with significant pile-ups.
Abstract Information

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Principal Investigator(PI):* Vicky Kalogera
PI Department:* Physics and Astronomy
Abstract Title:* The Advent of Big-Data Astronomy: Supernovae and the Time-Variable Universe
Computational Resources:* Quest

Abstract:

Stripped-envelope supernovae (SNe) represent a challenge to our understanding of massive star evolution. Wind mass loss and binary interactions are the leading candidates to explain observations. The latter has gained support in the recent years with growing evidence that mass-loss rates due to line-driven winds are, in reality, 2 - 3 times lower. In this poster, I will focus on a class of SNe known as Type IIb SNe. These initially exhibit strong Hydrogen spectral lines but they weaken and disappear over time and are thought to arise from progenitors that have retained a small amount of their Hydrogen envelope. They are also the only class of stripped-envelope SNe with identified progenitors. Thus they are powerful tools for testing our understanding of massive stellar evolution. To identify possible evolutionary pathways to Type IIb SNe, we use Modules for Experiments in Stellar Astrophysics (MESA) to model a large population of single and binary star sequences covering a broad parameter space with a wide range of component masses and initial orbital periods and identify those that undergo core-collapse with 0.01 to 0.5 solar masses of residual Hydrogen envelope. We find no single star Type IIb progenitors in the parameter space covered. However, we do find a few binary Type IIb progenitors. In the future, I would like extend my analysis to model evolutionary pathways to other stripped-envelope SNe types. Such an analysis can be used to build a database recording properties of progenitor sequences and can aid in expediting classification, progenitor identification in pre-supernova images and further detailed follow-up and study. It will be an important tool in analyzing the wealth of data on the transient sky that will be available in the future with the advent of rapid-cadence big-data telescopes like the LSST.
Abstract Information

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PI Department:* Chemical and Biological Engineering
Abstract Title:* Catalytic Activity of Palladium- and Platinum-Oxide Nanoclusters Grown in Nanoporous Materials for Natural Gas Conversion
Computational Resources: * Quest

Abstract:

Current environmental concerns and the rising cost of fossil energy are motivating the search for efficient conversion processes that produce low cost fuels and release lower carbon dioxide emissions. Due to its escalating production, natural gas is likely to become one of the main sources of carbon-based chemicals in the next century. Natural gas consists mainly of methane and higher hydrocarbons such as ethane and propane. Because these molecules are not highly reactive, there are great challenges in selectively transforming natural gas components into more valuable chemicals, and this creates new opportunities for developing catalytic materials that can directly convert natural gas into useful products.

As part of the Inorganometallic Catalyst Design Center (ICDC), we seek to bridge the gap between heterogeneous and homogeneous catalysis and introduce a new class of cluster catalysts that combine the advantages of both fields. Metal-organic frameworks (MOFs) offer a promising platform for this task. MOFs are thermally-stable, attractive supports for well-defined, isolated active sites that have the potential to catalyze the conversion of light hydrocarbons found in natural gas. Their high porosity and surface area are ideal for facilitating the catalytic reaction between active sites and reactants.

With these incentives in mind, we are investigating the hydrogenation of ethylene using well-defined transition-metal-oxide nanoclusters that could be formed through atomic layer deposition (ALD) inside porphyrin-containing MOFs. Hydrogenation and dehydrogenation are among the key reactions envisioned for the transformation of shale-oil hydrocarbon gases into valuable chemicals and fuels. We predict palladium- and platinum-oxide nanoclusters to be potential candidates for catalyzing the hydrogenation of ethylene, and have studied their catalytic activity through first principle calculations. The results and continuation of this study will lead to a better understanding of the catalytic process and provide guidance for experimental efforts to find the optimal catalyst for natural gas conversion.
Polycystic ovary syndrome (PCOS) is a complex genetic disease affecting 6-10% of premenopausal women worldwide. Analogous to other complex diseases, common genetic susceptibility variants for PCOS account for less than 5% of the observed heritability. This deficit in heritability may be due to rare genetic variants with larger biological effects. We performed whole genome sequencing on 64 two-generation families (average size = 4.3 individuals), including 87 women diagnosed with PCOS, to determine whether rare genetic variants in particular genome regions may contribute to disease pathogenesis. Optimal call quality score and read depth thresholds were determined by examining results across four biological replicates. Variants were filtered for consistency with Mendelian inheritance and predicted deleteriousness. Associations between sets of rare variants and PCOS and its quantitative hormonal traits were assessed using gene-level and sliding windows burden tests, accounting for relatedness. After correcting for multiple testing (P(adj)), variants in the CAMKMT gene (2p21) were found to be significantly associated with dehydroepiandrosterone (DHEAS) levels (P(adj)=0.015). No genes were significantly associated with PCOS status or with fasting insulin or sex hormone binding globulin or testosterone levels. Variants in two additional loci, 9q22.32 and 10q22.3, and were found to be significantly associated with DHEAS (P(adj) = 0.020, 0.039, respectively) using the whole genome sliding windows approach, but these variants were limited to a relatively small subset of families. Our results suggest that rare variants occurring in a specific set of genes are not broadly responsible PCOS pathogenesis, but it remains possible that the deficit in heritability in PCOS may be due to private mutations in different genes in each of the families, resulting in convergent phenotypes, or that rare variants in certain gene sets may contribute to pathogenesis within different PCOS subpopulations. CAMKMT should be investigated further for its association with DHEAS levels and potential role in PCOS.
Abstract Information

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Abstract Title: * N/A
Computational Resources: * Quest and Vault

Abstract:

On September 14th 2015, the advanced Laser Interferometer Gravitational-wave Observatory (aLIGO) made the first direct observation of gravitational waves and opened a new field of observational astronomy. However, being the most complicated and sensitive experiment ever undertaken in gravitational physics, aLIGO is susceptible to various sources of environmental and instrumental noise that hinder the search for more gravitational waves.

Of particular concern are transient, non-Gaussian noise features known as glitches. Glitches can mimic true astrophysical gravitational waves, occur at a high enough frequency to be coherent between the two detectors, and generally worsen aLIGO’s detection capabilities. The proper classification and characterization of glitches is paramount in optimizing aLIGO’s ability to detect gravitational waves. However, teaching computers to identify and morphologically classify these artifacts is exceedingly difficult.

Human intuition has proven to be a useful tool in classification problems such as this. Gravity Spy is an innovative, interdisciplinary project hosted by Zooniverse that combines aLIGO detector characterization, citizen science, machine learning, and social science. In this project, citizen scientists and computers will work together in a sybiotic relationship that leverages human pattern recognition and the ability of machine learning to process large amounts of data systematically: volunteers classify triggers from the aLIGO data stream that are constantly updated as aLIGO takes in new data, and these classifications are used to train machine learning algorithms which proceed to classify the bulk of aLIGO data and feed questionable glitches back to the users.

In this poster session, I will show the workflow and initial results of the Gravity Spy project with regard to aLIGO’s future observing runs and highlight the potential of such citizen science projects in promoting nascent scientific fields to the general public.
Abstract:

Granular rocks deformed under laboratory conditions exhibit complex pressure dependent stress–strain responses and strain localization processes. Such class of quasi-brittle materials is in fact characterized by various forms of fine-scale heterogeneity, which generate macroscopic patterns that can be traced back to a range of micro-structural processes, such as crack initiation; crack propagation along complex three-dimensional paths; interaction and coalescence of distributed multi-cracks into localized continuous cracks; and interactions between fractured and unfractured material. While usual constitutive approaches describing the macro-scale response of porous rocks neglect such rich variety of microscopic processes, discrete numerical models allow the incorporation of material heterogeneity directly at the scale where such processes take place. This poster presents a new computational tool for the analysis of inelastic processes in granular rocks subjected to varying levels of confinement. The purpose is to provide a flexible and efficient computational tool for the analysis of failure processes in geomechanical settings. The proposed model is formulated within the frame of Lattice Discrete Particle Models (LDPM), which is calibrated to capture the behavior of a porous rock widely tested in the literature: Bleurswiller sandstone. It is shown that the model allows one to explore the effect of heterogeneous microstructures on the development of pervasive faulting and strain localization. Most notably, it is discussed how LDPM analyses can be interpreted from a macroscopic perspective, deriving a detailed description of inelastic deformation patterns at the continuum scale. It is further discussed how the combined use of LDPM analyses, continuum modeling, and bifurcation theory can enable one to assess predictive capabilities and limitations of the usual elastoplastic models for sandstones, thus suggesting possible enhancements of their formulation.
Abstract Information

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Abstract Title: * N/A
Computational Resources: * Computation at Argonne National Laboratory

Abstract:

Metabolomics is a burgeoning field in systems biology, as it provides a small-molecule-centric view of a cellular system that is largely orthogonal to enzyme- or gene-centric views provided by other ‘omics datasets. For this reason, metabolomics has great potential to drive the discovery of novel chemistry and pathways that have, to date, eluded discovery by other approaches. Today, the major bottleneck preventing the broader use of metabolomics data in systems biology is the identification of metabolites from their characteristic mass spectra. This process largely relies on incomplete biochemical databases, which biases studies towards rediscovery of known compounds and ensures that new metabolites and pathways are seldom discovered in untargeted studies.

To address this challenge, we have constructed Metabolic In silico Network Expansions (MINEs) that expand existing databases by using expert curated reaction rules to propose novel metabolites and reactions. The reaction rules include an enzymatic set, which has been demonstrated to reproduce a large fraction of known biochemical reactions and a set describing spontaneous (non-enzymatic) chemical transformations of metabolites under physiological conditions.

The resulting MINE databases are freely accessible for noncommercial use using a web application at http://minedatabase.mcs.anl.gov and via client APIs in Javascript, Python and Perl. The databases contain over 750,000 putative metabolites; over 90% of which are not found in PubChem, the largest freely available database of chemicals. MINEs have been used to annotate novel metabolites from 4 diverse organisms and we are using these predictions to inform our exploration of the reactions that damage labile metabolites and the mechanisms by which this damage is repaired or preempted. MINE databases are designed to shine a light on unannotated enzymatic functions and undiscovered metabolic pathways, enabling more complete and predictive models of cellular systems.
Abstract Information

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Abstract Title: * Fully resolved simulations of esophageal transport based on the immersed boundary method.
Computational Resources: * Quest

Abstract:

Esophageal transport is a complicated mechanical and physiological process that transfers the ingested food bolus from the pharynx to the stomach through a multi-layered esophageal tube. The process involves the interactions among a bolus, esophageal wall composed of mucosal, circular muscle (CM) and longitudinal muscle (LM) layers, and the neurally coordinated muscle activation including CM contraction and LM shortening. In this work, we present a 3D fully-resolved model of esophageal transport based on finite-element/finite difference coupled immersed boundary method. Specifically, we adopt finite element method to describe the continuum-based esophagus model. We use finite difference method to describe the incompressible Newtonian flow for the bolus. We develop a simple mechanical model to mimic the neurally-controlled muscle activation wave. We first show a base case that corresponds to the normal physiology, and analyze the deformation and stress of esophageal wall as well as transport characteristics and compare with available experimental results. We then simulate cases with different muscle activation wave to study the influence of neural disorder. We also simulate cases with varying muscle fiber architecture observed experimentally to understand the roles of muscle layers. Finally, we present our preliminary study on bolus emptying based on a new esophageal-gastric model. To our best knowledge, those are first fully-resolved computational models on esophageal transport. Those simulation-based studies provide insights that are not easily obtained from experiments, and help to advance the knowledge on human physiology and pathophysiology related to the digestive system. Those simulation-based models also pave the road for future patient-specific diagnosis and treatment, and hold the potential to guide the development of related artificial organs.
Abstract Information

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Abstract Title: * A Genome- and Phenome- wide Study of Diverticulosis
Computational Resources: * Quest and Vault

Abstract:

Summary: The exploding growth of available genetic data coupled with longitudinal electronic health records (EHRs) enables the phenome-wide association studies (PheWAS) to discover novel phenotype associations for genetic variants. By performing PheWAS on the diverticulosis patients of the eMERGE cohort, we demonstrate its feasibility as a novel tool for not only exploring novel genotype-phenotype associations but also providing a comprehensive catalog of human diseases associated with published variants.

Introduction: Genome-wide Association Studies (GWAS) have evolved over the decades into powerful tool for exploring the genetic basis of human disease, providing hypothesis-free investigation of the whole genome. However, GWAS have limited ability to identify clinically significant variants, and account only for a portion of the predicted phenotypic heritability. As a complement to GWAS, phenome-wide association studies (PheWAS) have been developed, which can offer insights into the biological mechanisms that predict one’s susceptibility to disease, and help to determine promising polymorphisms or variants for further study.

Method: As part of the eMERGE network, we developed and validated a phenotype extraction algorithm to find cases and controls for diverticulosis and diverticulitis, using Natural Language Processing (NLP) technique. We performed GWAS of diverticulosis cases, the subset of those with diverticulitis, and controls, selected using EHR data from all adult eMERGE subjects. We selected the top SNPs associated with diverticulosis, and diverticulitis for the PheWAS on the eMERGE adult cohort of ~38,000 individuals.

Results: The GWAS found 39SNPs to be highly correlated (p>10^-8) with either diverticulosis and/or diverticulitis. Subsequent PheWAS identified several significant associations with skin disorders and vitamin deficiency, which correlations are already suggested by recent epidemiologic studies. As a disease of epithelial cells, the correlation of the SNPs associated with diverticulosis and skin disorders is biologically plausible and may suggest a possible disease pathway.
Abstract Information

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PI Department:* Mechanical, Civil and Environmental Engineering
Abstract Title:* Tunable biomaterials: tailoring point mutations to customize protein adhesion
Computational Resources: * DOD – High performance computing cluster. Keten Group Dynano Cluster

Abstract:

Curli fibers are functional amyloid protein assemblies that are a main constituent in the extracellular polymeric substance of enteric bacterial biofilms and serve a key role in bacterial cell adhesion and attachment to surfaces. Although understanding infection, biofouling, and creating bioinspired adhesives necessitates explaining curli’s contribution to adhesion, their interactions with surfaces and the molecular mechanisms governing these are not fully understood. Furthermore, these robust fibers are capable of self-assembly with added mutations or conjugations, which can affect bulk biofilm mechanical properties.

Here, we use Molecular Dynamics to investigate the interaction between individual curli monomers and substrates with varying chemistry, and how these are affected by incorporating mutations in the monomer. We find that both structural features and residue-specific features govern adhesive strength. While flexible turn and terminal regions facilitate adhesion to both surfaces studied, preferential interactions to a surface depend on residue chemistry (through electrostatic interactions) and geometry (through van der Waals interactions). We believe the diverse array of residue features within the curli fiber allows strong adhesion to various surfaces. Furthermore, considering the role of flexibility in adhering to a surface, we investigate the propagation of structural changes throughout the monomer structure. We find that certain clusters of residues exhibit correlations in flexibility or motion, and the perturbation of some residue positions induce changes that propagate throughout the monomer. Results regarding residue-surface interactions and correlated motion of certain sequence positions are then used to select point mutation type and position to tune adhesion to a surface. Finally, we present preliminary findings testing mutations aimed at customizing adhesive strength.
Abstract Information

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PI Department:* Biostatistics, Preventive Medicine and Applied Math (ESAM)
Abstract Title:* Network-Based Identification of Driver Genes in Expression Data
Computational Resources: * Quest

Abstract:

Genome-wide high-throughput assays generate large sets of data that must be carefully analyzed to elucidate the mechanisms that underlie a given phenotype. Specific disease-associated genes that can be targeted therapeutically have classically been identified by testing each gene for significant differences in expression between cases and controls. However, because this approach excludes information about gene regulatory networks, it can miss genes that are in fact crucial drivers of the given phenotype. While current pathway and network-based analyses incorporate systems-level information, their capabilities are limited to identifying whole pathways rather than specific genes that can be targeted therapeutically. To bridge this gap, we present a novel analysis technique that incorporates systems-level information, in the form of a network model of cellular interactions, with expression data to identify the genes that control disease-associated mechanisms. Based on our network-based analysis of expression data from a gene perturbation experiment, we hypothesize that these "mechanistic driver" genes will be correlated with neighbors in the network and that nearby genes will exhibit greater differential expression. We have devised a computationally efficient method that identifies genes that match this signature. Using a curated set of publicly available ovarian cancer data, we show that our method identifies genes missed by the classical approach. Our novel analysis approach complements existing gene-- and pathway-- based analysis strategies to identify specific genes that control disease-associated pathways, providing a new strategy for identifying promising therapeutic targets.
Abstract Information

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PI Department:* Department of Materials Science and Engineering
Abstract Title: * First Principles Investigation of Rechargeable Battery Cathode Material
Computational Resources: * Quest and NERSC

Abstract:

Alternative next-generation battery technologies beyond the current lithium-ion battery technology that are more efficient, cost-effective, and clean have received attentions recently. During the past decade, density functional theory (DFT), a computational quantum mechanical modelling method developed by Kohn and co-workers, brought a rapidly growing impact on battery materials research, where it can predict the ground state energy, intercalation voltage profile, phase diagram, and electronic structure of the crystal structure that can be used as an electrode. We have first investigated the Mn-based cathode materials (e.g. LiMn2O4 and Li2MnO3), which are more attractive cathode candidates for emerging applications such as electric vehicles (EVs) because of its low cost and abundance. By computationally modeling the spinel LiMn2O4 surface structures, we are able to provide a novel strategy to suppress Mn dissolution and the Jahn-Teller distortion associated with Mn3+, which has been a challenging task to overcome in order to mitigate capacity fading in the Mn-based cathodes. Furthermore, we design new Li-rich cathode compounds with a high-throughput DFT strategy in collaboration with battery scientists at Argonne National Laboratory, by screening among thousands of existing and hypothetical compounds with desired properties. Beyond the conventional lithium-ion technology, we have also presented dual-salt Mg2+/Li+ batteries that can discharge in as fast as 2 min with remarkable capacity retention. We have conducted extensive theoretical investigations to reveal the underlying mechanism, which we show that there is a threshold Li+ activity for the pristine Mo6S8 cathode to prefer Li+ insertion instead of Mg2+. Our current computational materials research can offer significant impacts in the energy storage and conversion research field and be also particularly appealing to the general public, media, and government agencies since we live in the era where people interact with a rechargeable battery on a daily basis from the smartphones and tablets, to emerging EVs.
Abstract Information

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Abstract Title:* Recoverable Slippage Mechanism in Multilayer Graphene Leads to Repeatable Energy Dissipation
Computational Resources: * Quest

Abstract:

Understanding the deformation mechanisms in multilayer graphene (MLG), an attractive material used in nanodevices as well as in the reinforcement of nanocomposites, is critical yet challenging due to difficulties in experimental characterization and the spatiotemporal limitations of atomistic modeling. In this study, we combine nanomechanical experiments with coarse-grained molecular dynamics (CG-MD) simulations to elucidate the mechanisms of deformation and failure of MLG sheets. First, a CG-MD model of MLG is established using a strain energy conservation approach, which is able to quantitatively reproduce MLG’s mechanical response in the elastic and fracture regimes as well as the superlubricity effect. Second, elastic properties of graphene sheets with one to three layers are measured using film deflection tests. A nonlinear behavior in the force vs deflection curves for MLGs is observed in both experiments and simulations: during loading/unloading cycles, MLGs dissipate energy through a “recoverable slippage” mechanism. The CG-MD simulations further reveal an atomic level interlayer slippage process and suggest that the dissipated energy scales with film perimeter. Moreover, our study demonstrates that the finite shear strength between individual layers could explain the experimentally measured size-dependent strength with thickness scaling in MLG sheets. This combined experimental and computational method can be extended to understand other low-dimensional materials, such as boron nitride, molybdenum disulfide and so forth.
Abstract Information

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PI Department:* Psychology
Abstract Title: * Silent lip reading generates speech signals in auditory cortex
Computational Resources: * Hardware Grant: nVidia GPU

Abstract:

Visual lip movements improve auditory speech perception in noisy environments1 and crossmodally activate auditory cortex2. However, it remains unclear what specific information about lip movements is relayed to auditory cortex. We demonstrate that the observation of lip movements generates neural activity in auditory cortex similar to that generated while listening to phonemes. We recorded electrocorticographic (ECoG) activity from macroscopic depth electrodes implanted within primary/secondary auditory cortices of the brains of two epilepsy patients. On each trial patients were presented with one of four representative auditory phonemes (/ba/, /da/, /ta/, and /tha/) or videos showing the lip movements articulating those phonemes, visemes. We constructed an ensemble of deep convolutional neural networks to determine whether the identities of the four phonemes (from auditory trials) and visemes (from visual trials) could be decoded from auditory cortical activity. Reliable decoding of viseme identity would provide evidence of coding of visual lip movements in auditory cortex. We first verified that heard phonemes were reliability decoded from activity in auditory cortex. Critically, seen visemes were also reliably decoded from activity in auditory cortex, indicating that visual lip movements generate viseme-specific activity in auditory cortex in the absence of any sound. Importantly, the classifier trained to identify visemes successfully decoded phonemes with comparable accuracy, indicating that the patterns of activity in auditory cortex evoked by visemes (from lip movements) were similar to those evoked by auditory phonemes. These results suggest that visual lip movements crossmodally activate auditory speech processing in a content-specific manner.